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CHEMICAL & ENGINEERING NEWS
MARCH 13, 2017

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Three stories about how molecules are made
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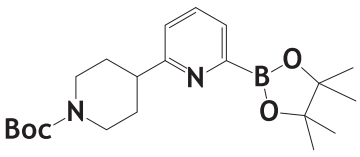
Novel Heterocyclic Intermediates for Cross-coupling Reactions



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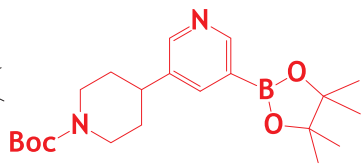

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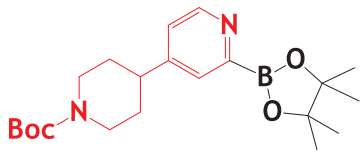

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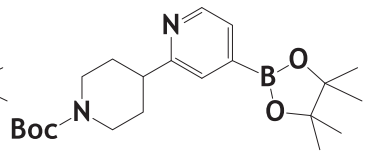

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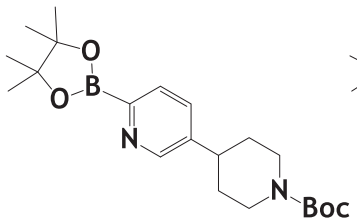

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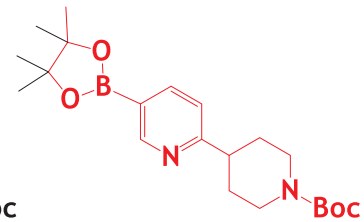

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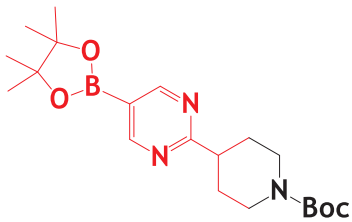

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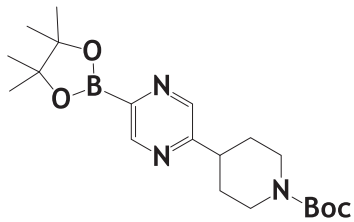

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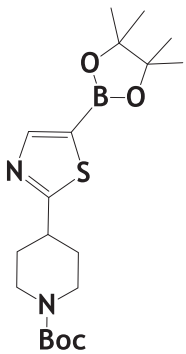

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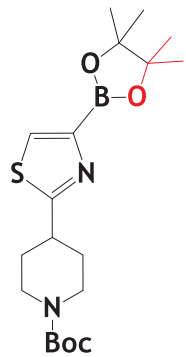

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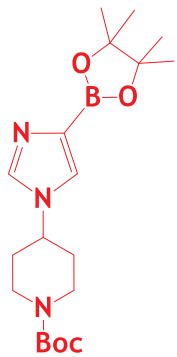

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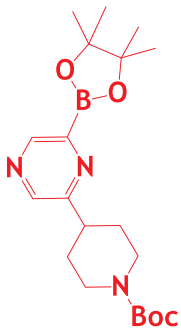

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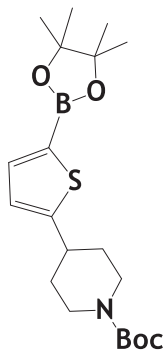

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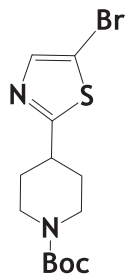

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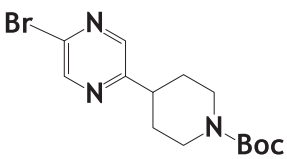

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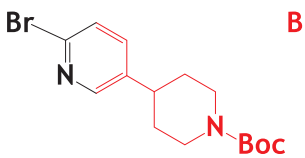

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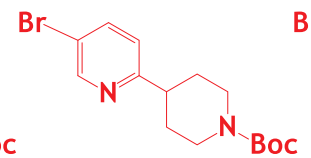

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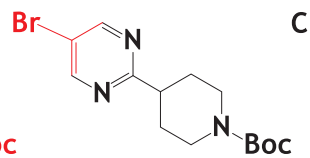

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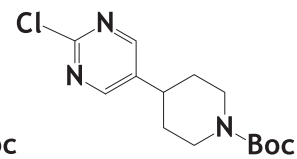

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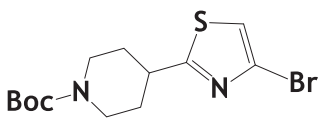

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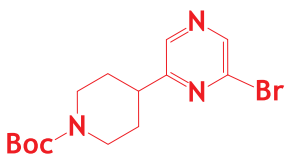

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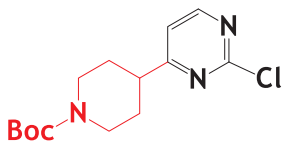

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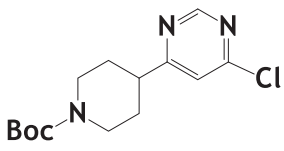

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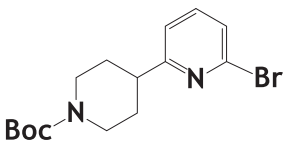

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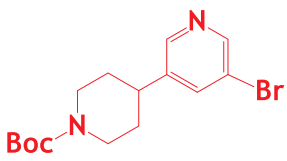

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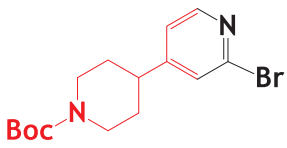

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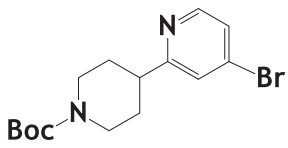

CS6639

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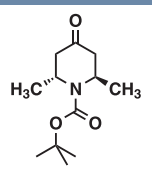

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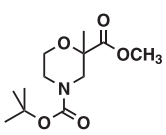

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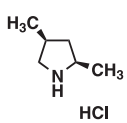

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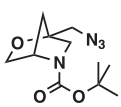

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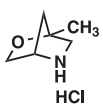

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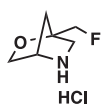

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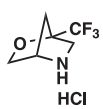

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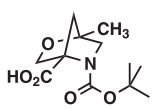

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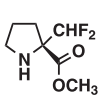

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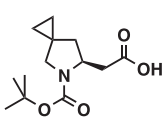

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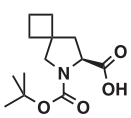

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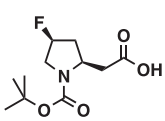

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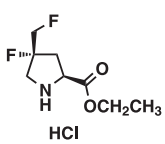

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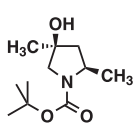

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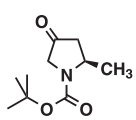

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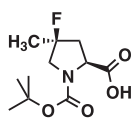

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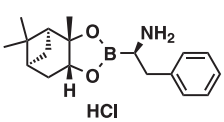

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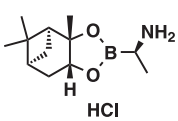

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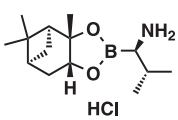

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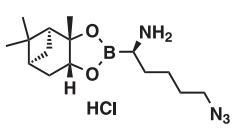

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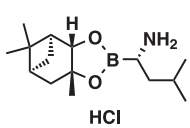

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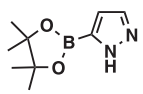

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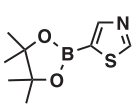

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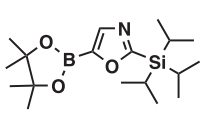

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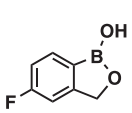

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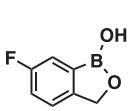

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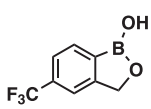

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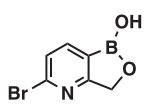

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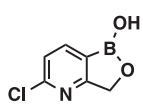

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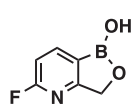

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OmegaChem Inc.
480 Rue Perreault
Levis, QC G6W 7V6
CANADA
orders@omegachem.com

BoroChem PBO
10 rue du professeur Zarifian
14200 Hérouville Saint Clair
FRANCE
sales@borochem.fr

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On the cover
Illustration by Yang H. Ku/ C&EN/Shutterstock

Quote of the week

"Electrosynthesis represents a disruptive technology and will be a game changer for industry."

—Siegfried R. Waldvogel, professor, Johannes Gutenberg University Mainz **Page 23**

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1155—16th St., N.W., Washington, DC 20036
(202) 872-4600 or (800) 227-5558

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Published by the **AMERICAN CHEMICAL SOCIETY**
Thomas M. Connelly Jr., Executive Director & CEO
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Canadian GST Reg. No. R127571347
Volume 95, Number 11

From the Editor

Live from Pittcon

I recently returned from attending Pittcon in Chicago. The annual conference and exposition on laboratory science took place March 5–9, and as we have come to expect from events of this size, it offered a little something for everyone: a packed technical program, workshops, poster sessions, awards, short courses, and plenty of networking opportunities.

Keep an eye out in the coming weeks for in-depth reports about the latest research and trends in analytical chemistry and instrumentation by C&EN reporters Marc Reisch and Celia Arnaud. To whet your appetite, here are a few nuggets of what happened during the show.

From the technical program, it is worth highlighting the keynote lecture by Howard Hughes Medical Institute investigator and Stanford University professor Karl Deisseroth. He spoke about the rapidly expanding field of optogenetics, in which scientists modify specific cells in the nervous systems of lab animals so that they respond to light. This allows researchers to use light to explore how stimulating specific neural circuits may affect the behavior of animals—how they interact with each other and their surroundings, how they move. Deisseroth is a pioneer in this field, and aptly, he was part of the group that helped launch then-president Barack Obama's BRAIN Initiative in 2013. The initiative, which is ongoing, was designed to support the development and application of technologies that will help scientists better understand brain function and improve how we can cure, treat, and prevent its disorders.

Another familiar face in the lecture program, and also focusing on the brain, was *Analytical Chemistry* Editor-in-Chief Jonathan Sweedler of the University of Illinois, Urbana-Champaign. His talk covered the development of analytical tools that allow cell-by-cell characterization in the brain. Sweedler discussed the advancements made in single-cell profiling using mass spectrometry techniques that can be performed on large cellular populations. Such methods allow researchers to sample thousands of cells at the same time and identify some of the most important—not necessarily abundant—metabolites in them. Understanding how neurons use these chemicals to talk to each other and what role they play during learning or how they affect memory or different human behaviors is crucial to begin to address brain conditions such as mental illness or addiction.

Besides Deisseroth and Sweedler, other speakers taking part in the technical program were Nobelist W. E. Moerner from Stanford University, Shana Kelley from the University of Toronto, and Chad Mirkin from Northwestern University.

On the exhibition floor, Pittcon's live demos proved very popular. Now in their second year, they included dynamic image analysis systems designed to extract information about a sample's particle size and shape; ultrasensitive mass spectrometers that could analyze the air at the show in real time and identify trace organic compounds; and portable Raman detectors for real-time monitoring of chemicals through white plastic containers, colored glass bottles, or manila envelopes. These demonstrations were limited in terms of the scope of what was possible (for example, there was no running water available), but they were entertaining and educational and were particularly suited to showcase portable technology. A fun addition, although it was unclear how it was connected to analytical chemistry or Pittcon, was the Lego gravity car racing, where attendees could build cars and then compete with each other.

For C&EN, an exciting moment was when as part of the awards program, another familiar face, 2016 Talented 12 winner Renã Robinson from the University of Pittsburgh, was recognized with the Pittsburgh Conference Achievement Award. We'd like to congratulate her on this accolade. Which reminds me: Keep nominating for this year's T12 class at cenm.ag/t12nom.

The deadline is April 1.

Editor-in-chief
@BibianaCampos

Views expressed are those of the author and not necessarily those of ACS.

Concentrates

Chemistry news from the week

Highlights

INFECTIOUS DISEASE

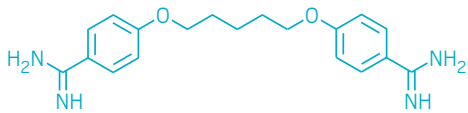
Dual therapy first weakens, then kills antibiotic-resistant pathogens

The drug pentamidine disrupts the outer membrane of Gram-negative bacteria, allowing antibiotics inside to finish the job

Among the most nefarious human pathogens are bacteria with two sets of membranes protecting their innards. The doubled armor can prevent antibiotics from penetrating these so-called Gram-negative bacteria, and it can help them develop resistance to antibiotics. Now a team led by Eric Brown at McMaster University has found a way to weaken the outer membrane of Gram-negative microbes so that previously unusable drugs can penetrate and kill the pathogens—including several multi-drug-resistant strains (*Nat. Microbiol.* 2017, DOI: 10.1038/nmicrobiol.2017.28).

In late February, the World Health Organization published a list of our planet's most problematic bacterial pathogens. The top three are multi-drug-resistant Gram-negative microbes from the *Acinetobacter* and *Pseudomonas* genera and Enterobacteriaceae family. They can cause life-threatening pneumonia or systemic infections, and patients are increasingly acquiring them in hospitals. As a last resort, doctors can treat infected people with antibiotics that are toxic to nerve and kidney cells. But bacteria are developing resistance to even these suboptimal drugs, threatening "to cause a serious breach in our last line of defense against multi-drug-resistant Gram-negative pathogens," Brown explains.

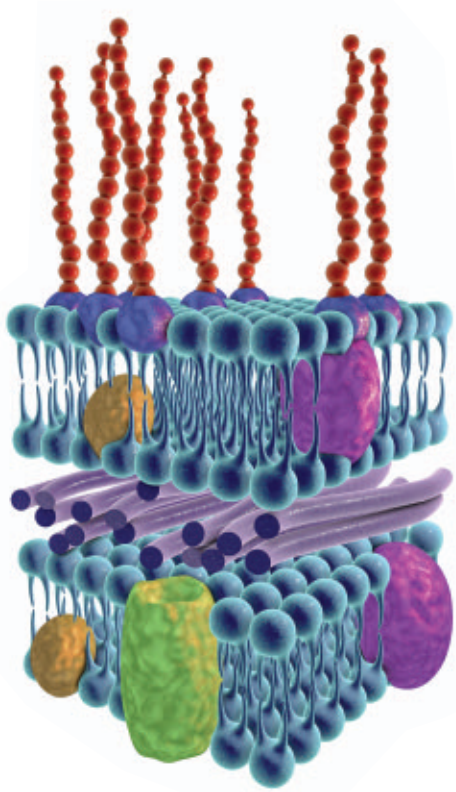
To tackle this problem, Brown and colleagues looked for compounds that disrupt the outer membranes of Gram-negative bacteria. They found an existing drug, pentamidine, which doctors often use to kill the protozoan pathogens that cause sleeping sickness and leishmaniasis.



Pentamidine

After infecting mice with multi-drug-resistant *Acinetobacter baumannii,* the team could cure the animals by administering a combination of pentamidine and antibiotics for Gram-positive pathogens, bacteria with only one membrane.

"Pentamidine can breathe life into drugs we don't usually use for Gram-negative infections because they wouldn't have been able to cross the outer membrane," comments Robert Hancock, a University of British Columbia microbiologist who characterized Gram-negative pathogens early in his career and now focuses on battling antibiotic resistance. "And another exciting thing is that pentamidine is already a drug," he adds. So there's a possibility it could be fast-tracked by regulatory agencies such as the Food & Drug Administration because it's already been proved safe in humans.



Pentamidine helps disrupt the outer membrane of Gram-negative pathogens, allowing antibiotics inside to do their work.

The new work supports a growing belief among scientists that developing compounds to weaken rather than kill bacteria can lessen pathogens' evolutionary drive to become resistant. Once weakened, the pathogens can be killed with a drug that wouldn't otherwise work. "The idea," Brown adds, "is to add an agent to take care of a resistance mechanism, or in this case, to get around intrinsic resistance."

But to date, Brown says only one success story for this strategy in the clinic comes to mind: bacteria that are resistant to antibiotics with a β-lactam ring in their structure (a family of broad-spectrum drugs that includes penicillin). These antibiotic-resistant bacteria have enzymes that break down the ring structure. So doctors prescribe β-lactamase inhibitors—weakening agents—along with β-lactam antibiotics to kill the pathogens.—SARAH EVERTS

CREDIT: SHUTTERSTOCK

OBITUARIES

George Olah dies at 89

Nobel Laureate advanced carbocation chemistry and alternative-energy technology

George A. Olah, the Donald P. and Katherine B. Loker Distinguished Professor of Organic Chemistry at the University of Southern California and the recipient of the 1994 Nobel Prize in Chemistry, has died. He was 89.

Olah was a towering figure, physically and scientifically, who earned international chemistry fame 40 years ago for his novel use of "magic acid," a concoction of antimony pentafluoride and fluorosulfonic acid that is billions of times as strong as sulfuric acid, to prepare long-lived carbocations.

By extending the lifetimes of these fleeting species, Olah was able to probe them directly via spectroscopy methods. That work rapidly advanced and greatly popularized the study of reactive intermediates and organic reaction mechanisms. It ultimately led to Olah's receipt of the Nobel Prize.

In addition to research in fluorine chemistry, Olah and longtime USC colleague and scientific collaborator G. K. Surya Prakash recently focused on the chemical transformations needed to convert methane and carbon dioxide to methanol. They aimed to drive the so-called methanol economy, in which an inexpensive, abundant, and carbon-neutral supply of methanol could be widely used as an energy carrier.

In the drive to develop technology that underpins methanol use, the USC researchers developed a direct methanol fuel cell for generating electricity from methanol without first producing hydrogen. The team also developed catalytic processes for reducing the greenhouse gas carbon dioxide to methanol.

In an industrial development of this green technology, Carbon Recycling International began operating the world's first commercial CO_2-to-renewable-methanol plant in Iceland in 2012. Named in Olah's honor, the plant recycles 5,500 tons of CO_2 annually and produces some 5 million L of methanol, which is used in gasoline blends.

Upon winning the ACS Priestley Medal, Olah remarked that other than the Nobel, no award meant more to him than the ACS Award in Petroleum Chemistry, which he received in 1963 for his work on Friedel-Crafts chemistry related to refinery processing of crude oil.

Olah, who in 1963 had recently relocated from Hungary, said: "I was an unknown immigrant at that time. And for a young guy who came from a faraway country and started all over with nothing, it really was a significant honor." ACS later renamed the award the George A. Olah Award in Hydrocarbon or Petroleum Chemistry.

"He was an amazing guy—a visionary and a giant of a chemist," says Prakash, who worked with Olah for more than 40 years. "He was also a great mentor and teacher, always jovial and very friendly."

Gabor A. Somorjai of the University of California, Berkeley, knew Olah since the 1950s, when they were both at the Technical University of Budapest. "George was a tireless promoter of science and technology, especially connected to energy independence," Somorjai says. "He used his scientific talents and excellent communication skills for the benefit of society."

The University of Utah's Peter J. Stang, another fellow Hungarian chemist, expresses a similar sentiment: "George was one of the most creative and original chemists of the 20th and early 21st centuries," Stang says. "The world has lost a great person and a great scientist in the truest sense of the word."—MITCH JACOBY

PHYSICAL CHEMISTRY

Quantum effect could explain chiral interactions

Electron spin polarization dictates recognition between chiral compounds

Biomolecules from small amino acids to large DNA helices are chiral, and how they interact depends on their chirality. A newly identified quantum effect could help explain how biomolecules' chirality persists.

When two molecules interact, their electron clouds reorganize. In chiral molecules, that reorganization is accompanied by electron spin polarization that enables molecules of the same chirality to interact more strongly than molecules of opposite chirality, reports a research team led by Ron Naaman and Jan M. L. Martin of the Weizmann Institute of Science and David H. Waldeck of the University of Pittsburgh (*Proc. Natl. Acad. Sci. USA* 2017, DOI: 10.1073/pnas.1611467114).

"The mechanism that they have demonstrated is different from any that was previously reported," comments David N. Beratan of Duke University. "If the idea holds up, it could entirely change the way we think about molecular recognition in biological and organic chemistry."

In the new work, Naaman and colleagues combined experimental studies of helical oligopeptides with computational analysis. They found that the electron spin polarization induced by molecular interactions constrains the symmetry of the wave functions involved in the interactions. The symmetry constraints in turn lead to energy differences when molecules of the same chirality interact compared with molecules of opposite chirality, favoring homochiral interactions.

"It's a real quantum mechanical property that can't be represented in classical-physics-based models," Naaman emphasizes.

The effect is short-range and arises only when electrostatic and other noncovalent interactions bring molecules together, making it more likely to influence enantiospecific recognition in a crowded cellular environment than in dilute solutions. It is also additive and becomes more significant when many chiral functional groups interact across the surfaces of large biomolecules.—JYLLIAN KEMSLEY

CREDIT: MITCH JACOBY/C&EN

Data bit stored on single atom

Lab demo may lead to strategies for boosting data-storage density

In the drive to cram ever more information into handy data-storage devices, researchers have reduced the size of a bit of data to the ultimate limit—a single atom (*Nature* 2017, DOI: 10.1038/nature21371). The study may lead to ways of increasing the data-storage density of devices such as computer hard drives, in which information is encoded in magnetic materials.

To store data on a computer hard drive, a device known as a read-write head rapidly magnetizes nanometer-sized regions of the hard disk. That process sets the magnetic polarities of these domains, or bits, in one of two states, corresponding to the zeros and ones of digital data. The head reads the data by sensing the magnetic state of the domains.

For decades, hard-disk manufacturers have been increasing their devices' data-storage densities by gradually shrinking the size of the magnetic domains in which data are stored. One challenge has been ensuring that the microscopic domains are magnetically stable. If the polarity of a domain spontaneously flips, data will be lost. That problem is related to the domains' composition and size, as well as their thermodynamic properties.

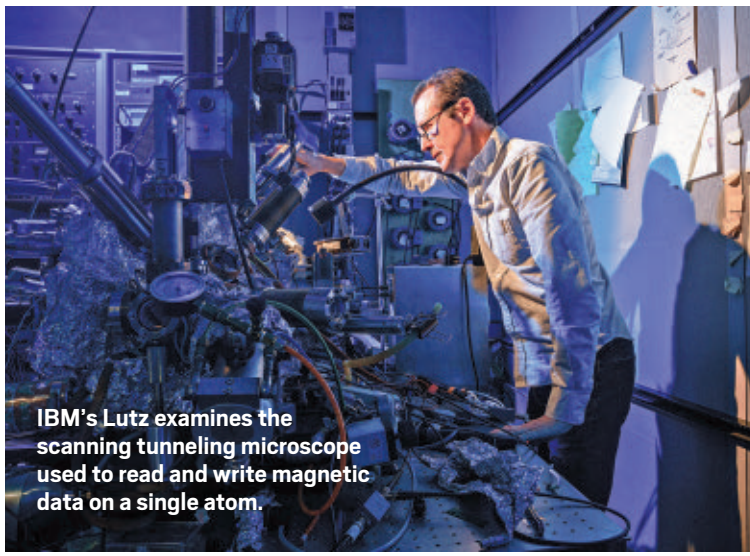
The domains in today's commercial devices, which have lateral dimensions in the nanometer range and are a few atomic layers thick, typically consist of hundreds of thousands of atoms. Meanwhile, various researchers have continued to shrink that bit size to just a handful of atoms in lab demonstrations.

Now, that number has been reduced to just one atom by Fabian D. Natterer, Christopher P. Lutz, and coworkers at IBM Almaden Research Center.

By using a custom-made scanning tunneling microscope (STM) at ultralow temperatures and under ultrahigh vacuum, the team isolated a few holmium atoms on a magnesium oxide film and applied brief electric pulses to set the atoms' magnetic states, or spins. Then the team detected the orientation of the spins via an STM technique known as tunnel magnetoresistance, which showed that the spins can be switched at will and remain stable for several hours. To confirm that they had achieved spin switching, the researchers placed one iron atom near the holmium atoms and used it as a magnetic sensor in a single-atom electron spin resonance measurement.

Describing the experimental techniques at the heart of the study as "ingenious," Roberta Sessoli, a specialist in magnetic materials at the University of Florence, asserts that the IBM team has "unambiguously achieved the ultimate limit of writing and reading information."

The complexity of the method means that the work is still far from real-world applications, she notes, yet it shows that it is possible to store and retrieve magnetic information with a single atom.—MITCH JACOBY



IBM's Lutz examines the scanning tunneling microscope used to read and write magnetic data on a single atom.

CREDIT: IBM RESEARCH ALMADEN

C–H ACTIVATION

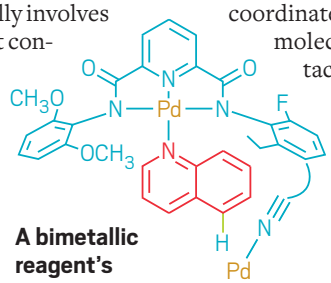
Enzyme-inspired route to heterocycle functionalization

Bifunctional metal agents reversibly coordinate heterocycles and derivatize them at remote sites

Chemists often use C–H activation to help replace specific hydrogen atoms in organic compounds with complex functional groups. This strategy generally involves covalently bonding a reagent containing a C–H-activating group, such as a palladium atom, to a substrate that already has a directing functional group. The directing group steers the C–H activator to the desired C–H bond. Once the bond breaks, a new functional group replaces hydrogen and the directing group is removed.

A new class of bimetallic reagents now uses enzyme-inspired reversible metal coordination, instead of covalent bonding, to achieve C–H activation and functionalization in nitrogen heterocycles, with no need to preinstall or later remove a directing group. The reagents, designed by Jin-Quan Yu and coworkers at Scripps Research Institute California, also activate remote C–H bonds that have been difficult to reach or completely inaccessible with other synthetic techniques (*Nature* 2017, DOI: 10.1038/nature21418).

C–H activation hasn't worked well with heterocycles because metal activators tend to coordinate with heteroatoms, interfering with site selectivity. Yu and coworkers have now turned that problem into an advantage. In their new bimetallic reagents, one palladium atom is designed intentionally to coordinate reversibly with the heteroatom of a substrate, positioning the second metal to activate a remote C–H bond.



A bimetallic reagent's anchoring palladium (near center) coordinates with the nitrogen atom of a substrate (quinoline in this case, red), positioning the reagent's second palladium (lower right) to activate a remote C–H bond (green).

The reagents use distance and geometry constraints to focus on specific target sites on substrates, like enzymes do. They coordinate reversibly with substrate molecules, derivatize them, detach after activation, and then move on to activate other substrate molecules, also like enzymes do. The reagents work stoichiometrically or catalytically, and relatively large amounts are required. But their efficiency can potentially be improved, experts say.

Yu and coworkers used the new reagents to alkenylate a range of nitrogen heterocycles, including phenylpyridine, quinoline, and the anticancer natural product camptothecin, none of which could previously be functionalized in the same way using C–H activation, Yu says.

Motomu Kanai of the University of Tokyo comments that the technique is "very powerful," noting that it could ease drug design by making it possible to modify compounds at positions other methods cannot easily reach. Victor Snieckus of Queen's University in Ontario calls the discovery "a major leap forward in synthetic aromatic substitution chemistry." And Kian Tan, who leads the Chemical Technology-Synthesis group at Novartis in Cambridge, Mass., says the templates are amazingly well designed and versatile, making it "easy to envision creating libraries of templates to access different selectivity patterns."—STU BORMAN

> The discovery is "a major leap forward in synthetic aromatic substitution chemistry."
>
> **—Victor Snieckus,** Queen's University in Ontario

CREDIT: SHUTTERSTOCK

FOSSIL FUELS

Refining a crude analysis

Method improves crude oil separation, could aid petrochemical refining and spill assessment

Crude oil is an unruly soup of tens of thousands of organic compounds, and this diversity makes it difficult to pick out individual molecules from the crowd for analysis using standard tools such as mass spectrometers. Despite the vast quantities of crude oil used globally each day, much remains unknown about its chemical composition, which can vary dramatically from one oil field to the next.

A method that separates crude oil into a dozen fractions based on their chemical properties now promises more details about composition: It could help chemists measure low levels of molecules that corrode pipelines or pinpoint the most toxic compounds in an oil spill (*Anal. Chem.* 2017, DOI: 10.1021/acs.analchem.6b04202).

Fractionation is not a new approach to simplifying oil analysis. One of the most common methods, dubbed SARA, uses chromatography to split oil into four broad classes: saturates, aromatics, resins, and asphaltenes. But this separation is based largely on the molecules' solubilities in the solvent being used, and many chemical classes remain obscured within the mélange in each fraction.

In contrast, the new method developed by Steven J. Rowland of the University of Plymouth and coworkers is particularly good at teasing apart a mixture of polar compounds containing nitrogen, sulfur, or oxygen—often responsible for poisoning oil-processing catalysts—which conventional analytical methods struggle to identify.

The procedure is not based on radical innovation. It relies on a series of columns filled with commercial ion exchange resins and silica, making the method reproducible, relatively simple, and inexpensive. "The real novelty is putting it all together," says Ryan P. Rodgers, director of the Future Fuels Institute at Florida State University, who was not involved with the work. By deploying the separation columns in the right order and eluting the crude oil with a series of increasingly polar solvents, the method isolates molecules depending on how well their functional groups stick to each type of column. This process yields fractions that are each dominated by a particular chemical class: sulfoxides, quinolines, carbazoles, fluorenones, and more.

After analyzing each fraction with techniques such as gas chromatography/mass spectrometry, the team identified dozens of specific compounds. Some of them, such as thioxanthones, were previously unknown in crude oil. The method achieves "a better separation between different classes of chemicals," says Sonnich Meier of the Institute of Marine Research. "It's the best I've seen."

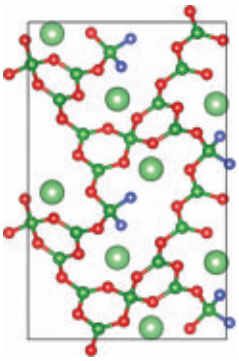
Meier has been working with Rowland's team for the past three years and plans to use the technique to single out the compounds in crude oil that are toxic to fish embryos, which can be contaminated during an oil spill.

Meanwhile, the oil industry increasingly wants to know the precise composition of a crude oil before investing in extracting it. Declining production of low-sulfur, sweet crude, oil has the industry relying on heavier crudes requiring more refining and posing greater risks of pipeline corrosion or blockages.—MARK PEPLOW, special to C&EN

MATERIALS

▶ Nonlinear optical laser material avoids beryllium

Materials scientists have developed a new class of deep-ultraviolet nonlinear optical (DUV NLO) crystals that promise to be less toxic and have better performance than the materials currently used (*Angew. Chem. Int. Ed.* 2017, DOI: 10.1002/anie.201700540). DUV NLO materials are increasingly being used in the semiconductor industry and are crucial in producing solid-state lasers with wide frequency ranges. The fluorooxoborate $KBe_2BO_3F_2$, which is the only practical laser material for generating light below 200 nm, has had researchers scrambling for alternatives to avoid further use of toxic beryllium. It also grows in layers, which can reduce its optical properties. Now, a team led by Shilie Pan, vice director of the Chinese Academy of Science's Xinjiang Technical Institute of Physics & Chemistry, has prepared a class of beryllium-free fluorooxoborate crystals that don't layer. The team's strategy involved inserting $(BO_3F)^{4-}$, $(BO_2F_2)^{3-}$, or $(BOF_3)^{2-}$ groups into three-dimensional boron-oxygen networks. The material works as needed without beryllium, and the synthesis method avoids the formation of terminal oxygen atoms—the existence of which leads to layer formation. One compound in particular, $Li_2B_6O_9F_2$, promises to further "break down the DUV wall for NLO materials," the researchers report.—ELIZABETH WILSON



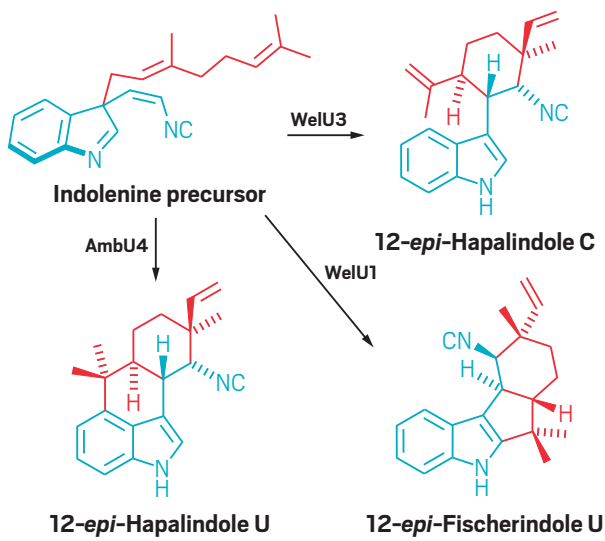
$Li_2B_6O_9F_2$ offers deep-ultraviolet nonlinear optical properties without beryllium and debilitating layering.

BIOCATALYSIS

▶ Indole alkaloid biosynthetic pathways unraveled

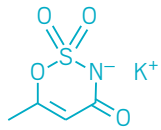
Indole-based alkaloid natural products such as fischerindoles and hapalindoles have promising antimicrobial and antitumor activities, but they are difficult to make synthetically. New findings on how cyanobacteria biosynthesize them could help guide future synthetic efforts. Xinyu Liu and Qin Zhu at the University of Pittsburgh have discovered that U-protein enzymes catalyze cascade reactions that structurally diversify a common precursor into different indole alkaloids (*Chem. Commun.* 2017, DOI: 10.1039/c7cc00782e). For example, three of the enzymes—WelU1, WelU3, and AmbU4—convert a single indolenine into a tetracyclic fischerindole, a tricyclic hapalindole, and a tetracyclic hapalindole, respectively. Each enzyme's cascade reaction includes a Cope rearrangement, an aza-Prins cyclization, and a carbocation-deposition

The enzymes AmbU4, WelU1, and WelU3 use cascade reactions to convert a common indolenine precursor into three natural products.



ENVIRONMENT

Sweetener tracks tinkling in the pool



Acesulfame potassium

Researchers estimate that swimming pools contain 30 to 80 mL of urine for each person who's jumped in. The problem, aside from the ick factor, is that urine reacts with chemical disinfectants in the water to form potentially harmful by-products. To track the safety of pools and hot tubs, scientists would like to find a chemical marker of how much urine is actually in the water. Xing-Fang Li and coworkers at the University of Alberta propose that the artificial sweetener acesulfame potassium—used in products such as beverages and baked goods, often in combination with other sweeteners—could be that marker. Humans don't metabolize the sweetener, so it's excreted intact in urine. Li and coworkers used liquid chromatography and tandem mass spectrometry to measure acesulfame in 250 samples from 31 pools and hot tubs in two Canadian cities. They also sampled the corresponding input tap water for comparison (*Environ. Sci. Technol. Lett.* 2017, DOI: 10.1021/acs.estlett.7b00043). The team found the sweetener in all pool and hot-tub samples at concentrations from 30 to 7,110 ng/L, compared with 15 ng/L or less in the tap water samples. Using the average amount of acesulfame in a human urine sample, the researchers then estimated that urine can account for up to 30 L of the volume in a standard 420,000-L community pool. The ubiquity of acesulfame suggests that it could indeed be used as a urinary marker for tracking water quality, the researchers note.—CELIA ARNAUD

CREDIT: SHUTTERSTOCK (POOL); *ANGEW. CHEM. INT. ED.* (CRYSTAL STRUCTURE DIAGRAM)

step. The indolenine precursor and its derivatives are structural isomers, so the cascades in effect are multistep rearrangements. With U-protein enzymes now in hand—they can be isolated from cyanobacteria—Liu believes it will be easier to synthesize diverse members of this family of bioactive natural products in the laboratory.—STU BORMAN

CHEMICAL COMMUNICATION

Bumblebees leave foot odor on flowers

Not only do bumblebees have smelly feet, but the insects also leave an imprint of their foot odor on flowers they visit. In fact, the hydrocarbon chemical signature is so strong that it can be detected for about 24 hours after being deposited. A team of researchers led by Richard F. Pearce of the University of Bristol reports that bumblebees visiting flowers can also decipher whether the left-over foot funk is their own, a nest mate's, or that of an entirely unknown bumblebee. The researchers think being able to distinguish these odor prints could prevent bees from making redundant visits to the same nectar source (*Sci. Rep.* 2017, DOI: 10.1038/srep43872). Bumblebees aren't the only insects to leave behind smelly foot residues as they go about their day: Wasps, termites, and ants also secrete mixtures of hydrocarbons from their feet that give each individual its own personal aroma. The secretions also help with adhesion and with avoiding desiccation. For bumblebees, their signatures often include (*Z*)-9-tricosene and other long-chain hydrocarbons, and the relative concentration of these components uniquely identifies an individual. The new findings represent the first time researchers have been able to show that bumblebees can distinguish their odor from that of their nest mates, Pearce notes.—SARAH EVERTS

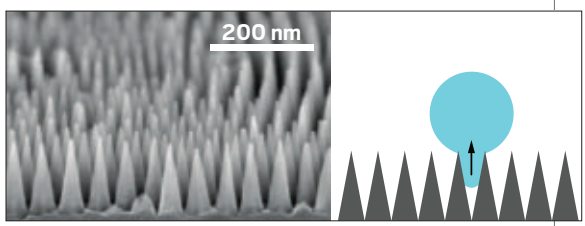
When bumblebees land on a flower, they leave behind their foot odor, which stems in part from (*Z*)-9-tricosene (shown).

CREDIT: *NAT. MATER.* (CONES); SHUTTERSTOCK (BEE)

NANOMATERIALS

Nanostructures lift the fog

To state the obvious, water makes things wet. What may not be so obvious, however, is that even superhydrophobic surfaces can succumb to water's propensity to moisten. Researchers often fashion tiny hydrophobic bumps, pillars, and protrusions on these surfaces to help keep water away. But they've found that fine fog droplets can still slip into the spaces between nanostructures and accumulate into larger drops to wet surfaces. So researchers led by David Quéré of ESPCI Paris launched a systematic investigation into the design of nanotextured hydrophobic surfaces that get around the fogging problem (*Nat. Mater.* 2017, DOI: 10.1038/nmat4868). By plasma etching self-assembled thin films of a polystyrene-poly(methyl methacrylate) block copolymer, the team created arrays of rods or cones, depending on the etching conditions. The researchers then coated the arrays with hydrophobic fluorinated chlorosilane groups. Water droplets initially grew on all the textured surfaces, but substrates with tightly packed cones eventually kicked the droplets off. The shape and proximity of the cones caused growing droplets to contort dramatically, which generated enough pressure to expel water from the surface with unprecedented efficiency, Quéré explains. He adds that such droplet departure has been observed previously, but "what seems unique with nanocones is the rate of departure is much, much larger than previously reported." Understanding this behavior could help scientists design better antifogging windshields, mirrors, and solar cells, the researchers say.—MATT DAVENPORT

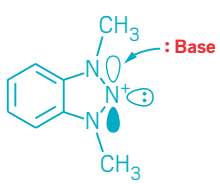


Hydrophobic nanocones pinch the bottom of fog droplets, creating enough pressure to eject the water from the surface and prevent fogging.

CHEMICAL BONDING

Nitrogen Lewis acids unveiled

Lewis acids and bases are one of chemistry's fundamental concepts, depicting a molecule's ability to accept an electron pair from a partner molecule or to donate an electron pair to a partner, respectively. For example, electron-rich nitrogen-centered molecules such as ammonia function as Lewis bases. Mark Gandelman of Technion—Israel Institute of Technology and his group have found a situation in which they can turn that donor-acceptor reactivity around, so that a nitrogen-centered molecule functions as a Lewis acid (*J. Am. Chem. Soc.* 2017, DOI: 10.1021/jacs.6b12360). Gandelman's group had previously studied a triazolium salt and found it to be an analog of imidazole-based N-heterocyclic carbenes, including the ability to serve as a ligand for transition metals. The central nitrogen of the saturated N–N–N triazolium unit in the molecule can accept electron density from a metal into a vacant p orbital, even though it weakly donates its lone pair of electrons residing in an sp^2-type orbital to the metal. With that information in hand, the team decided to treat various triazolium compounds with different Lewis bases such as phosphides, phosphines, and carbanions and found that the nitrogen-centered molecules functioned as the Lewis acid partner. Gandelman and coworkers think these new nitrogen-based Lewis acids could join other well-established Lewis acids based on boron, phosphorus, aluminum, and tin and serve in reactive frustrated Lewis pairs or other types of catalysts.—STEVE RITTER



Triazolium Lewis acid

COATINGS

Rejecting PPG bid, AkzoNobel will exit chemicals

Proposed merger would be latest consolidation move for industry

AkzoNobel has rejected an unsolicited takeover offer from PPG Industries and says it will instead embark on a program to separate its specialty chemical business from its main business in paints and coatings.

PPG privately proposed on March 2 to acquire AkzoNobel in a deal that would value the Dutch company at about $22 billion. AkzoNobel says it rejected the proposal as not in the interests of its stakeholders.

PPG says it will consider its path forward. AkzoNobel's stock rose more than 15% after the disclosures, indicating that investors are betting PPG will come back with a higher offer.

PPG and AkzoNobel each have annual sales of roughly $15 billion. And the two companies have done business before. In 2013, PPG acquired AkzoNobel's North American decorative coatings business for about $1 billion.

Both companies are largely paint makers that also operate chemical businesses. Both have pared back their chemical operations—PPG through the sale of its chlor-alkali operations in 2012 and Akzo Nobel through the sale of its catalyst business in 2004.

AkzoNobel sells its Dulux paints in China.

Still, AkzoNobel continues to be a major player in chemicals, with a specialty chemical business that had sales of $5.1 billion last year. The company considers itself to have leadership positions in markets such as surfactants, polymer chemistry, pulp processing, and chlor-alkali.

According to AkzoNobel CEO Ton Büchner, PPG's bid "brought forward" a plan to separate the chemical business. Taking the step now will allow AkzoNobel to "unlock the value within our company ourselves" rather than submit to an acquisition that substantially undervalues the firm, he says.

Future options for the chemical business include establishing it as an independent company. PPG did not say if it intends to keep the chemical operation if it ultimately succeeds in its bid for AkzoNobel.

A successful PPG bid for all of AkzoNobel would continue a relentless wave of consolidation in the chemical and allied industries. Dow Chemical and DuPont are pushing to complete their historic merger by the end of the first half of the year. The industrial gas giants Praxair and Linde plan to merge. Bayer is advancing its acquisition of agricultural products rival Monsanto. And ChemChina is close to completing its acquisition of Syngenta.—MICHAEL MCCOY

BY THE NUMBERS

87%

The proportion of researchers using CRISPR who are new to gene editing, according to a survey by Synthego, a provider of synthetic RNA used in genome editing and research. Although CRISPR is viewed as easier to use than older gene-editing methods, the Synthego survey showed that a majority of users struggle with making edits efficiently, verifying the edits, and delivering genes.

BIOBASED CHEMICALS

Nestlé, Danone look to renewable bottles

Nestlé Waters and Danone are the latest beverage makers to investigate biobased polyethylene terephthalate (PET). They are teaming up with the California-based start-up Origin Materials to form the NaturALL Bottle Alliance, which hopes to have water bottles made from renewable PET on store shelves by 2020.

PET is typically made from the petrochemicals ethylene glycol and purified terephthalic acid (PTA). Since 2009, Coca-Cola has been using biobased ethylene glycol in its PlantBottle, but it and other companies have struggled to come up with an alternative to PTA derived from petrochemical *p*-xylene.

Origin was formerly known as Micromidas, which got its start with a fermentation process for converting municipal wastewater into polyhydroxyalkanoate.

In 2011, the firm licensed a technology from the University of California, Davis. Now Origin's main focus, the process uses hydrochloric acid to convert biomass into 5-chloromethylfurfural (CMF), which is reduced to 2,5-dimethyl furan. That undergoes a Diels-Alder reaction with ethylene to yield *p*-xylene via an oxanorbornene intermediate.

Nestlé and Danone invested in Origin as part of a $40 million financing round last fall. The company has received $80 million since its founding in 2008.

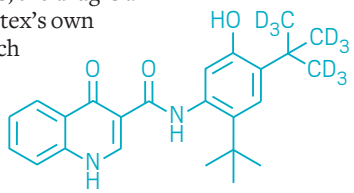
Origin has been running a pilot plant in Sacramento for three years. Next year, it plans to inaugurate a plant that can make about 10,000 metric tons of CMF per year, according to CEO John Bissell. The company hopes to open a plant 10 times that size in 2022.—ALEX TULLO

CREDIT: AKZONOBEL (PAINT CANS); NESTLÉ (BOTTLE)

PHARMACEUTICALS

Vertex buys Concert's cystic fibrosis drug

Vertex Pharmaceuticals will pay up to $250 million for Concert Pharmaceuticals' cystic fibrosis drug CTP-656. Currently in Phase II clinical trials, the drug is a deuterated version of Vertex's own compound ivacaftor, which it sells under the name Kalydeco.



CTP-656

Like ivacaftor, CTP-656 is a cystic fibrosis transmembrane conductance regulator (CFTR) potentiator. Substituting deuterium atoms for specific hydrogens in the structure generates a novel compound with altered pharmacokinetic properties. Notable is its longer half-life, which means CTP-656 may need to be given only once per day versus two times daily for Kalydeco.

For Concert, the deal validates its deuterium chemistry approach to drug design and presents an opportunity for CTP-656 to advance toward commercialization. Vertex already leads the cystic fibrosis drug market with Kalydeco and Orkambi, a CFTR potentiator combination it launched in 2015. Sales of the two products reached $1.7 billion in 2016.

Vertex will acquire rights to all of Concert's other cystic fibrosis research and preclinical programs. Concert intends to use the money to support itself through 2021 and advance its deuterated JAK 1/2 inhibitor CTP-543, now in Phase II testing to treat the autoimmune disease alopecia areata.

The deal brings at least three benefits to Vertex, Leerink stock analyst Geoffrey C. Porges told clients in a report. It removes a potential competitor, adds a new compound that can improve the firm's existing cystic fibrosis therapy combinations, and extends its intellectual property protection by at least five years.—ANN THAYER

AGRICULTURE

DSM, Evonik form omega-3 joint venture

DSM and Evonik Industries are setting up a joint venture to make omega-3 fatty acids from natural marine algae for use in fish feed and pet food.

The venture, called Veramaris, will spend $200 million to build an omega-3 fatty acid facility at an existing Evonik site in the U.S. It will go onstream in 2019. The firms have already made pilot-scale quantities of the oil at DSM's facility in Kingstree, S.C.

The new plant will turn out a "highly concentrated algal oil," the partners say, using algae production expertise from DSM and industrial-scale fermentation know-how from Evonik.

Veramaris plans to supply enough omega-3 fatty acid to meet 15% of the needs of the salmon farming industry.

Omega-3 fatty acids are a family of polyunsaturated fats that include eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA).

Initial output from the planned facility will meet about 15% of the farmed salmon industry's demand for EPA and DHA, the two firms say. Fish use omega-3 for metabolic functions and as a cellular membrane component.

Most of the omega-3 fatty acids used by the aquaculture industry today come from harvested wild fish such as sardines. A number of companies have developed alternative sources of protein for farmed fish, but finding an alternative source of omega-3 fatty acids has proven difficult until now, the partners say.

DSM and Evonik have had a joint technology development agreement since July 2015. Both companies say they achieved positive results in product development while "extensively working with the entire value chain, including fish feed producers, fish farmers, and retailers."—ALEX SCOTT

INFORMATICS

Instrument makers invest in cloud computing

Thermo Fisher Scientific has acquired Core Informatics, a fast-growing, venture-capital-backed provider of cloud-based scientific data management systems with about 100 employees.

Thermo Fisher announced the purchase last week at the Pittsburgh Conference on Analytical Chemistry & Applied Spectroscopy (Pittcon) in Chicago. It underscored the growing importance for instrument makers of systems capable of handling, storing, and manipulating the flood of data from today's scientific instruments.

"Their cloud-based offerings are more discovery oriented, while what we already had supported quality control and quality analysis in manufacturing processes," explained Dan Shine, analytical instruments president at Thermo Fisher. "They will integrate seamlessly into what we already have."

Also at Pittcon, Waters Corp. launched the cloud version of its Empower chromatography data management system. "The cloud has changed the way the world interacts with data," said Steve Smith, Waters' informatics vice president, by "allowing companies to focus on science and not the infrastructure."

Managing information through cloud-based software is part of PerkinElmer's strategy too, said Jim Corbett, head of the firm's discovery and analytical solutions unit.

Instruments are generating more data than they did just a few years ago, and scientists need a way to sort through it all, Corbett said. Cloud-based software systems make that possible, he noted. PerkinElmer made its own informatics acquisition with the purchase of laboratory software and services firm Ceiba Solutions in 2014.—MARC REISCH

CREDIT: DSM

BIOBASED CHEMICALS

Biobased start-up tries new financing route

Blue Marble Biomaterials aims to raise money via a stock offering to small investors. Based in Missoula, Mont., Blue Marble uses biorefining to convert food waste into chemicals. Last year it launched a dithiazine bacon flavor from raw materials such as coffee grounds, tomato pomace, and grape pomace. It also formed a collaboration with Welch's to upgrade waste from grape and apple juice processing. In 2015, the Securities & Exchange Commission adopted Regulation A+, which allows start-ups to raise up to $50 million from small investors. Previously, such venture capital investing was limited to high-net-worth individuals.—ALEX TULLO

ELECTRONIC MATERIALS

Sumitomo to triple OLED touch screens

Sumitomo Chemical will triple capacity at its South Korean subsidiary Dongwoo Fine-Chem to make film-based touch-screen panels for displays based on organic light-emitting diodes. The films are particularly suited for use on curved and flexible displays, Sumitomo says. The Japanese firm decided to expand its plant because South Korean display makers are significantly expanding. OLED displays are present on Samsung smartphones and may be adopted by Apple for its next generation of iPhones.—JEAN-FRANÇOIS TREMBLAY

The Samsung Galaxy Edge phone features an OLED display.

DRUG SAFETY

FDA warns Wockhardt, Fosun

The U.S. FDA has again warned the Indian generic drug producer Wockhardt about problems at one of its facilities, this time in the U.S. The agency also warned a subsidiary of Fosun Pharmaceutical—one of China's leading drug producers—regarding a facility in southwest China. In a statement to the National Stock Exchange of India, Wockhardt says FDA has banned its Chicago-based unit, Morton Grove Pharmaceuticals, which produces oral and topical formulations, from launching new products in the U.S. until it addresses manufacturing deficiencies. In December, FDA warned Wockhardt about failure to maintain sterile conditions and manufacturing data integrity at a facility in Gujarat, India. In China, FDA uncovered data integrity issues at Fosun's Chongqing Pharma Research Institute subsidiary, which produces active pharmaceutical ingredients. Investigators found that the firm deleted "entire chromatographic sequences" and other data from its computer records.—JEAN-FRANÇOIS TREMBLAY

START-UPS

BASF, others back P2 Science

The renewable chemical company P2 Science has closed a $9.6 million series B financing round that included BASF Venture Capital. The company says it will use the proceeds to build its first commercial plant, in the New Haven, Conn., area. Co-founded by Yale University, Yale scientists, chemical industry veteran Neil Burns, and Elm Street Ventures, P2 uses ozonolysis and flow chemistry to convert feedstocks such as vegetable oil and forestry-derived terpenes into specialty chemicals.—MICHAEL MCCOY

CLIMATE CHANGE

Alberta funds CO_2 to chemicals

The Alberta government will award a total of $12 million to four projects that seek to transform carbon dioxide from waste into an asset. Two of the projects, from Solidia Technologies and CarbonCure Technologies, sequester CO_2 by injecting it into concrete during the curing process. Mangrove Water Technologies, a spin-off from the University of British Columbia's chemical engineering department, is developing a reactor that converts CO_2 and saline wastewater into chemicals such as hydrochloric acid and carbonate salts. And working with the Canadian start-up Lumenfab, McGill University seeks to produce fuels from CO_2 and wastewater with the help of solar power.—MICHAEL MCCOY

SPECIALTY CHEMICALS

Fine Industries sold to Chinese buyer

The private equity firm Northedge Capital has sold the Middlesbrough, England-based fine chemicals firm Fine Industries to China's Lianhe Chemical Technology for an undisclosed sum. With 220 employees, Fine Industries had sales last year of $63 million and pretax profits of $12 million. It manufactures intermediates and active ingredients for pesticide and pharmaceutical customers along with a suite of specialty chemicals. Fine Industries was acquired by Degussa in 2001 before being sold to management in 2008 and then to Northedge in 2013.—ALEX SCOTT

COATINGS

Perstorp sells Belgium site to Synthomer

Swedish specialty chemical firm Perstorp has agreed to sell its site in Ghent, Belgium, which produces additives for the coatings industry, to England-based Synthomer for about $82 million. The plant has 45 employees and generated pretax profits of $8.5 million in 2016. "The business is an excellent

CREDIT: LESZEK KOBUSINSKI/SHUTTERSTOCK

fit and provides increased access to new products and customers," says Synthomer CEO Calum MacLean.—ALEX SCOTT

INORGANIC CHEMICALS

▶ Wacker will expand silicon in Norway

Wacker Chemie is expanding silicon metal capacity at its site in Holla, Norway. The company will spend about $90 million on a new plant that will come on-line in the first half of 2019. Wacker uses the metal to make silicones and polysilicon. The Holla plant currently covers one-quarter of the company's silicon requirements.—ALEX TULLO

BIOLOGICS

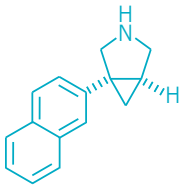
▶ China's BeiGene plans biologics plant

Beijing-based oncology drug discovery firm BeiGene is joining with the government of Guangzhou in southern China to build a $330 million biologic drug facility in the Guangzhou Development District. The venture will also fund biologic drug R&D in China. Under the agreement, $30 million will come from BeiGene and $150 million from Guangzhou. The venture will borrow the rest. BeiGene says it needs large-scale manufacturing facilities to ensure growth.—JEAN-FRANÇOIS TREMBLAY

MERGERS & ACQUISITIONS

▶ Otsuka to acquire Neurovance

Otsuka Pharmaceutical will pay $100 million up front and up to $150 million in potential milestone payments to acquire Cambridge, Mass.-based Neurovance, a six-year-old company focused on attention-deficit/hyperactivity disorder. Its lead ADHD candidate is centanafadine, which has completed Phase II clinical trials. According to Neurovance, centanafadine is one of a new generation of triple reuptake inhibitors that modulate the activity of norepinephrine, dopamine, and serotonin. The acquisition will extend Otsuka's efforts in the area of central nervous system therapy.—ANN THAYER



Centanafadine

ONCOLOGY

▶ Boehringer, Vanderbilt pact targets KRAS

Advancing a two-year-old cancer drug discovery partnership, Boehringer Ingelheim and Vanderbilt University will research and develop small molecules targeting a protein called SOS that acts as a molecular switch activating KRAS, a gene essential to normal tissue signaling. Mutations of the gene are responsible for the onset of various forms of cancer. The venture is based on research done in the laboratory of Vanderbilt chemist Stephen W. Fesik. The partners previously identified compounds that bind to KRAS with high affinity.—RICK MULLIN


A researcher in the Fesik lab at Vanderbilt.

CREDIT: VANDERBILT

VACCINES

▶ Sanofi, AstraZeneca in respiratory deal

Sanofi Pasteur and MedImmune, the biologics arm of AstraZeneca, have agreed to develop MED18897, a monoclonal antibody, for the prevention of lower respiratory tract illness caused by respiratory syncytial virus. MED18897 is currently in a Phase II clinical trial involving infants ineligible for Synagis, the current standard of care. Sanofi Pasteur will make an up-front payment of $127 million to MedImmune and milestone payments of up to $523 million.—RICK MULLIN

Business Roundup

▶ **Wacker Chemie** will spend about $7 million to expand silicone production at its Jandira site near São Paulo, Brazil. The firm says the project will boost output of antifoam compounds and specialty silicones for industries such as paper and personal care.

▶ **Vernalis and Servier**, partners since 2007, have set up a new two-year oncology drug discovery collaboration. Vernalis will receive an initial $2 million for applying its fragment- and structure-based drug discovery methods to the program.

▶ **Pharmaron**, a Beijing-based contract research firm, has agreed to buy a majority stake in a U.S. subsidiary of Japan's Shin-Nippon Biomedical Laboratories. Based at the University of Maryland BioPark, the subsidiary conducts Phase I and II clinical studies for drug industry customers.

▶ **Herbalife**, a producer of supplements used for weight loss and nutrition, has set up a 275-m^2 facility at the Bangalore, India, site of the contract research firm Syngene. Staffed with Syngene employees, the facility will help Herbalife formulate and test products for the Indian market.

▶ **Vaxess Technologies** has received two grants totaling about $6 million from the Bill & Melinda Gates Foundation to support the development of polio and measles-rubella vaccines. The company uses silk-derived biopolymers to create controlled-release microneedle patches for transdermal delivery of vaccines.

▶ **UCB Biopharma** has signed a multiyear "insourcing" agreement with the French contract research firm NovAliX. Under the pact, NovAliX will provide on-site chemistry services to support small-molecule drug discovery programs at Belgium's UCB.

▶ **BioVersys**, a Swiss biotech firm, will work with the U.S. drug discovery services firm Aptuit on new targets and molecules for Gram-negative bacteria. BioVersys studies small molecules that interfere with bacterial-resistance mechanisms.

▶ **Takeda Pharmaceutical** invested in the $120 million initial public offering of Arix Bioscience, a London-based firm that finances and builds life sciences businesses. Arix says it will create and incubate companies in partnership with Takeda.

CLIMATE CHANGE

EPA scraps methane reporting for oil and gas industries

Pruitt kills data collection at several states' request

The Trump Administration has withdrawn an EPA request that oil and natural gas companies provide information on their methane emissions from field operations.

The Obama Administration had sent the data request to some 15,000 oil and gas companies late last year. It asked for basic information on the numbers and types of equipment used at onshore drilling and production facilities as well as more detailed information on methane emission sources and control devices.

Earlier in 2016, EPA issued methane control regulations for new oil and gas facilities but did not address existing facilities. The data collection rule was an attempt by the Obama EPA to learn more about oil and gas operations in preparation for emissions regulations at operating facilities.

Oil and gas operations are the largest industrial source of methane, a greenhouse gas 25 times as potent as carbon dioxide, according to EPA.

The U.S. is experiencing an oil and gas bonanza, with some 1 million wells in operation. However, in the rush to exploit the resource, much is unclear—even the exact number of wells is uncertain. Confusion also surrounds the quantity of methane emissions. The now-canceled reporting was intended to help resolve this uncertainty.

"There is a lack of transparency in oil and gas operations," notes Mark Brownstein, vice president of climate and energy at the Environmental Defense Fund, an activist group. "We really don't know what is out there. You can't manage what you are not measuring. The irony is industry called for this information before EPA proposes to regulate existing oil and gas facilities."

"It is a missed opportunity," says Rob Jackson, a Stanford University earth scientist. Some companies are already collecting, and often sharing, information on their methane emissions, he adds.

Industry applauds the withdrawal. Howard Feldman, the American Petroleum Institute's director of regulatory affairs, calls EPA's announcement a "positive step."

EPA Administrator Scott Pruitt says the day before the March 2 withdrawal, he received a request from nine state attorneys general and the governors of Mississippi and Kentucky to kill the reporting request. EPA, he says, takes such concerns "seriously and is committed to strengthening its partnership with the states."—JEFF JOHNSON, special to C&EN

The Trump EPA nixed requirements for existing oil and gas operations to report their methane emissions.

CHEMISTRY IN PICTURES

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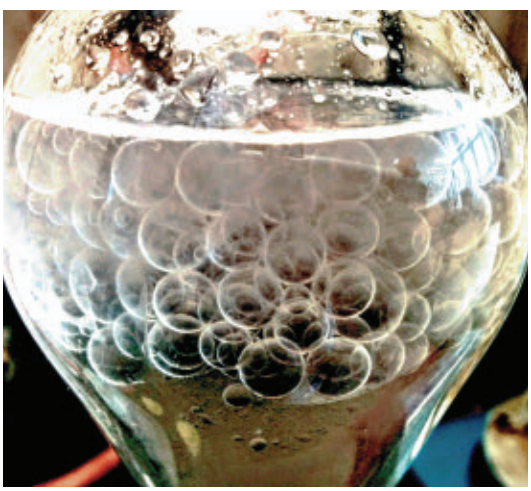


Liquids not playing nice

Maria Zakharova, a graduate student at Laval University, encountered this stunning emulsion when trying to purify the product of a reaction she'd run. She was trying to separate her low-polarity amide product from her reactant, undecanoic acid. Zakharova performed the extraction with dichloromethane (DCM), which dissolves her product, and water, which dissolves more-polar molecules, such as undecanoic acid. But instead of two clean, separable layers, Zakharova ended up with this. The undecanoic acid molecules anchored their polar heads in the water while keeping their nonpolar tails in the DCM, thereby forming micelles and preventing the water from settling as a separate layer. "This kind of emulsion remains stable for quite a long time—weeks, months," Zakharova says. "Even though this reaction looks beautiful, it is not easy to purify."—MANNY MORONE

Submitted by Maria Zakharova

CREDIT: ARINA P. HABICH/SHUTTERSTOCK (OIL JACKS)

NUCLEAR ENERGY

U.S. said to be falling behind in advanced reactors

The U.S. nuclear industry is lagging behind China, Russia, and others on advanced nuclear reactor technology because of regulatory hurdles, witnesses said last week at a Senate hearing. The U.S. is starting to cede its global leadership on nuclear energy, Ashley E. Finan, policy director of the research and advocacy group Nuclear Innovation Alliance, told the Senate Environment & Public Works Committee. With that leadership position goes "influence on nonproliferation discussions and on best practices and safety and on environmental issues globally," Finan said at the panel's hearing on the proposed Nuclear Energy Innovation and Modernization Act (S. 512). The bipartisan legislation, introduced earlier this month, is aimed at modernizing the U.S. nuclear regulatory process and revitalizing the nuclear industry sector, said Sen. John Barrasso (R-Wyo.), the committee's chair. Barrasso, who introduced the bill, is concerned that advanced nuclear reactor technology in the U.S. faces "delays and costs from regulatory red tape." The measure would require the Nuclear Regulatory Commission to develop a series of steps for licensing non-light-water reactors.—JESSICA MORRISON

BIOTECHNOLOGY

Prepare for flood of new products, report says

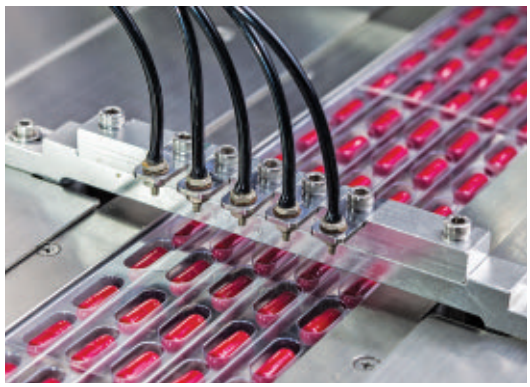
The U.S. regulatory system is likely to be overwhelmed by an onslaught of biotechnology products in coming years, according to a report from the National Academies of Sciences, Engineering & Medicine. In the report, the National Academies committee of academic and industry biotechnology experts recommends strategies to help federal agencies prepare based on predicted future biotechnology products and anticipated regulatory challenges. "The rate at which biotechnology products are introduced, and the types of products, are expected to significantly increase in the next five to 10 years, and federal agencies need to prepare for this growth," says Richard M. Murray, a Caltech bioengineering professor who chaired the committee. To be prepared, federal agencies should grow in-house expertise on the changing biotechnology landscape, coordinate cross-agency risk assessments for new products, and fund research into ethical, legal, and social implications of emerging biotechnology products, the report says. EPA, FDA, and USDA commissioned the study in 2015 as part of an effort to modernize the U.S. regulatory system for biotechnology products.—JESSICA MORRISON

CREDIT: SHUTTERSTOCK

PHARMACEUTICALS

U.S., EU to share pharma inspection reports

U.S. and European Union regulators have agreed to recognize each other's inspection reports of pharmaceutical manufacturing facilities. The decision is expected to help FDA and EU drug inspectors avoid duplicating inspections. It's also expected to lower inspection costs and help regulators focus resources in parts of the world where the risk of unsafe drugs is the greatest. The agreement comes after nearly three years of collaboration between FDA and EU inspectors to assess the risks and benefits of relying on foreign inspections of drug manufacturing facilities. Congress gave FDA the authority to use foreign drug inspection reports in 2012 with the passage of the FDA Safety & Innovation Act. The law allows FDA to recognize foreign inspections as long as those inspections meet U.S. requirements. "The Mutual Recognition Agreement is an important step in working collaboratively and strategically with key partners to help ensure that American patients have access to safe, effective, and high-quality drugs," says Dara Corrigan, FDA's associate commissioner for global regulatory policy.—BRITT ERICKSON



TRADE

Chemical sector outlines priorities for NAFTA rewrite

With the Trump Administration vowing to renegotiate the North American Free Trade Agreement with Mexico and Canada, trade groups representing the North American chemical industry say they are open to modernizing the accord. The American Chemistry Council, the Chemical Industry Association of Canada, and the Mexican Chemical Industry National Association say NAFTA has greatly benefited the industry, created jobs, and made the region more competitive globally. Trade in chemicals among the three NAFTA countries more than tripled from $20 billion in 1994 to more than $63 billion in 2014. But the groups say they are open to updating NAFTA, outlining priorities such as strengthening cross-border data protection, setting new standards for state-owned companies, and streamlining customs procedures. "Most importantly, all chemical products are traded duty-free under NAFTA, and a modernized NAFTA should maintain this policy," the industry associations say in a joint statement. It's unclear what changes the White House will seek in the trilateral trade agreement, but the GOP-led Congress is considering border adjustment import taxes and other measures that would upend the current tariff-free arrangement.—GLENN HESS, special to C&EN

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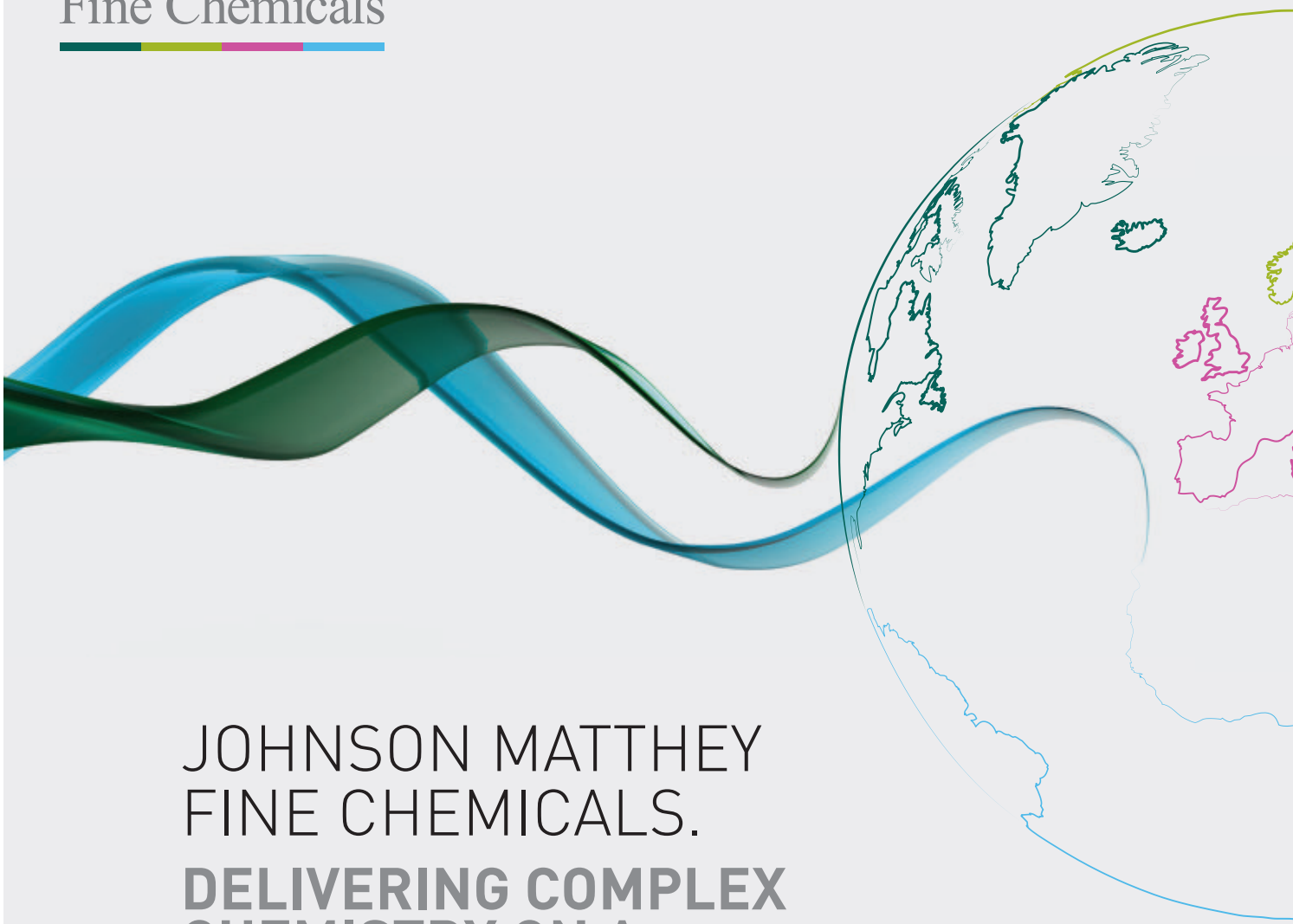

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Khademhosseini's lab at Harvard Medical School is diverse.

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EMPLOYMENT

Foreign students and postdocs in U.S. worry about the future

While Trump takes aim at immigration, foreign trainees consider taking their talents elsewhere

LINDA WANG, C&EN WASHINGTON

In late January, when President Donald J. Trump's initial executive order took effect barring people from seven predominantly Muslim countries from entering the U.S. for 90 days, the scientific community reacted swiftly (C&EN, Feb. 6, page 5). Among them, foreign graduate students and postdocs in the U.S. scrambled to figure out how such travel restrictions would affect them.

"The first 24 hours, nobody did any work," says Saghi Saghazadeh, an Iranian postdoc in the lab of Ali Khademhosseini at Harvard Medical School. "I was constantly refreshing news websites; that's all I did."

A federal judge issued a stay on that executive order, but President Trump on March 6 announced a new executive order that suspends for 90 days immigration from six, instead of seven, predominantly Muslim countries: Iran, Libya, Somalia, Sudan, Syria, and Yemen. Iraq, which was listed in the first immigration executive order, is no longer on the list.

These curbs on immigration are prompting foreign grad students and postdocs in the U.S. to consider alternative plans for their education and career, including moving to another country.

"I'm walking on eggshells, and I don't know what's going to happen," Saghazadeh says. "The worst part is that we cannot plan for the future."

The National Science Foundation's National Center for Science & Engineering Statistics conducts a Survey of Graduate Students & Postdoctorates in Science & Engineering. According to that survey, 45% of full-time graduate students in science and engineering in the U.S. were on a temporary visa in 2015.

Khademhosseini, who is researching tissue engineering, says the majority of students and postdocs in his lab are from other countries.

"We are very multicultural in our lab, and it's representative of most labs in the U.S.," he says. "I've always appreciated this vision of inclusiveness that the U.S. has had where if you work hard, you have the opportunity to do great no matter where you're from."

Khademhosseini, who is originally from Iran, says he's worried about the long-term impact these political actions will have on U.S. competitiveness in science and technology. "There are many places in the world that would love to have smart, educated people who have skills in science and technology," he says.

Khademhosseini and 45 other journal editors recently published an editorial in *ACS Nano* encouraging the scientific community to promote a culture of inclusiveness, tolerance, and diversity (2017, DOI: 10.1021/acsnano.7b00953).

Foreign grad students and postdocs whom C&EN spoke with said they are seriously considering leaving the U.S. for countries that have a more welcoming immigration policy. "I'm questioning staying in America, and I have already started looking through documents for Canada," Saghazadeh says. "I will go to a country where I have to worry less about my life."

Cathleen Crudden, a chemistry professor at Queen's University in Ontario and a member of C&EN's advisory board, says she has been fielding phone calls and e-mails every day from foreign scientists in the U.S. and other countries inquiring about joining her lab. "I've had people from the U.S. contact me to say that they want to

move in the middle of their Ph.D. program," she says. "That tells you how people are feeling, that they're willing to do that."

But just because a foreign grad student or postdoc moves to Canada doesn't guarantee an easier life. "The challenge in Canada is that we don't have the same capacity in terms of the workforce," Crudden says. "But that can always change. Most of the industry in Canada is made up of small multinational enterprises. But our government is interested in investing in science and technology. With growth and proper investment, we could certainly improve" the opportunities available in the chemical industry, she says.

The political uncertainty is discouraging foreign talent from heading to the U.S., whether for education, for work, or even just a scientific meeting. Grad students and postdocs who are from the affected countries worry that they won't be able to travel to the U.S. for conferences. Sogol Borjian, an Iranian scientist at Queens University, is program chair for an optical society conference in the U.S. in June, and she is not certain that she will be able to get a visa to attend. The American Chemical Society is hearing similar concerns from those scheduled to attend its national meeting in San Francisco next month.

Meanwhile, Sara Mahshid, an Iranian postdoc at the University of Toronto, says that because of the executive order, she was unable to attend a job interview at the University of California, Davis. She and her sister, Sahar, also a postdoc at the University of Toronto, are now wondering whether they should apply for jobs in the U.S. at all. "Even if I have a visa to enter the U.S., if I'm not eventually able to get a green card or a work permit, there is no point in offering someone like me a job," Sara Mahshid says.

It's not just students and postdocs from the affected countries who are feeling unsettled. A graduate student at Oklahoma State University who came to the U.S. from India in 2011 says he worries about potential changes that might happen to the process of obtaining an H-1B temporary work visa. He didn't want his name included out of concern for his career prospects.

On March 3, the Trump Administration announced suspension of expedited processing of H-1B visas for up to six months. And several bills now in Congress propose additional changes to the H-1B visa process.

For example, Rep. Zoe Lofgren (D-Calif.) has introduced the High-Skilled Integrity & Fairness Act of 2017, a bill designed to curb what some see as H-1B visa outsourcing abuse and instead attract highly skilled and highly paid workers. One portion of the bill deals with employers that are considered H-1B dependent—those that have at least 15% of their employees on H-1B visas.

With Lufgren's proposal, an H-1B-dependent employer would have to pay a certain percentage of its H-1B visa holders at least $130,000 annually to avoid restrictions regarding recruiting and displacing U.S. workers. That's a significant increase from the current H-1B-dependent wage exemption level of $60,000. What's more, the bill proposes a new formula to calculate the H-1B prevailing wage and allocation of H-1B visas.

"The bigger corporations would be in a position to be able to absorb those much higher wages, and they're hiring more computer programmers, computer engineers, and software engineers," says Brendan Delaney, an immigration lawyer with Leavy, Frank & Delaney in Bethesda, Md. "If you're a scientist on more of the research side of things, and a small or midsized biotech company wants to hire you, where are they going to be in all of this?"

The number of H-1B visas awarded to researchers in the chemical sciences is already extremely low. In 2015, according to data from the U.S. Citizenship & Immigration Services, initial H-1B petitions approved in occupations in mathematics and physical and life sciences accounted for approximately 4% of the total approved H-1B petitions. In comparison, 62% of the approved H-1B petitions went to computer-related occupations.

"If I get a job in the U.S., I would stay, but if I don't get a job, what am I going to do? I have to plan accordingly," says the Oklahoma State grad student. "I don't feel secure, and I don't have a clear vision of what's going to happen. I have to look at other options." He says he's looking into opportunities in Australia, New Zealand, Japan, and countries in Europe, as well as prospects back home in India.

Delaney points out that applying for an EB-1 "extraordinary ability" or an EB-2 "national interest waiver" green card is still an option for foreign scientists, although the bar for getting one of these green cards is high. "If you're good enough and you're accomplished enough, you can make a solid case," Delaney says. "At least there are still avenues open without having to be sponsored by companies." He encourages foreign scientists to educate themselves about the process so they know their options moving forward. At the ACS Career Fair at the society's national meeting in San Francisco in April, an immigration law firm will be available to answer questions about visas and other immigration issues. ACS will also be offering a workshop on navigating the U.S. visa process.

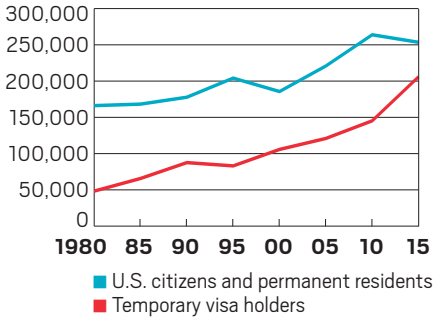
Foreign grad students and postdocs say they feel more isolated from their colleagues. "I'm the only person from one of the seven countries in my group," says Hooman Yaghoobnejad Asl, an Iranian postdoc at the University of Pennsylvania. "It somehow affects the way other people see you. Everyone is asking, 'So, what's going to happen to you next?' I feel like I've been separated from the group, and everyone is concerned about me."

Despite the political uncertainties, one thing is certain: "Scientists are learning to speak up," Khademhosseini says. "Many of the people I know who are scientists have never really been involved in activism and politics, but these kinds of things have made a lot more people aware, and they've started to think about how they can let their voices be heard," he says.

Saghazadeh agrees. "As international scientists we have always been closed in our labs, and we have not been communicating with people. That's why they see us as strangers," she says. "We should find a way to talk to people, and I hope we can get to a point where we can have a dialogue." ■

Foreign talent fills labs

The number of grad students in the U.S. who are on temporary visas is catching up to U.S. citizens and permanent residents.



Source: National Science Foundation's National Center for Science & Engineering Statistics

> "I don't know what's going to happen. The worst part is that we cannot plan for the future."
>
> —**Saghi Saghazadeh,** Iranian postdoc, Harvard Medical School

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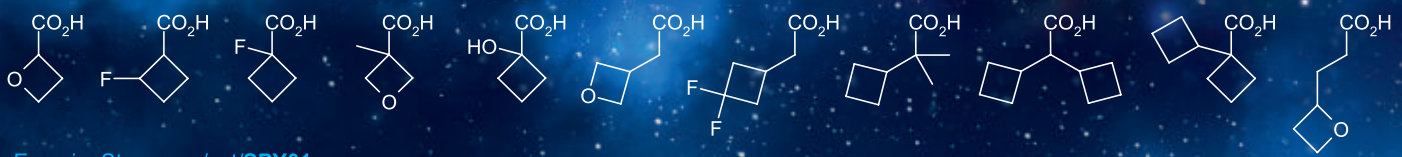

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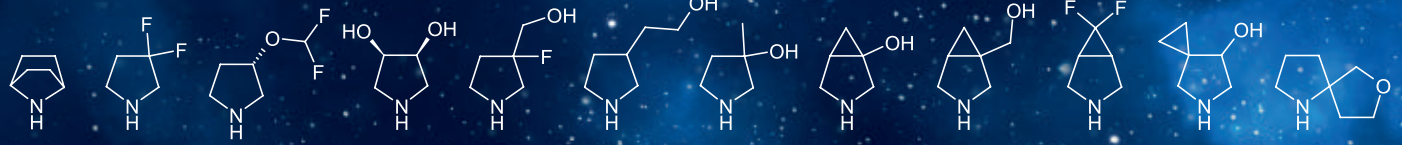

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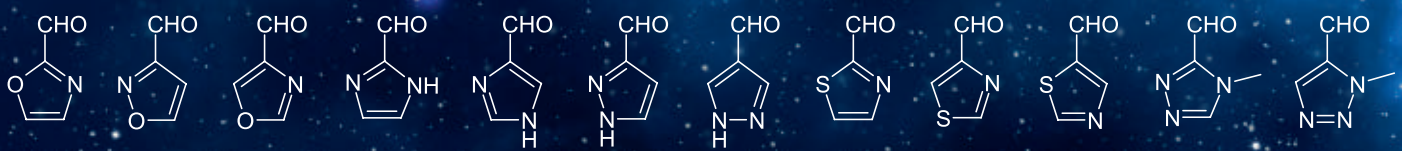

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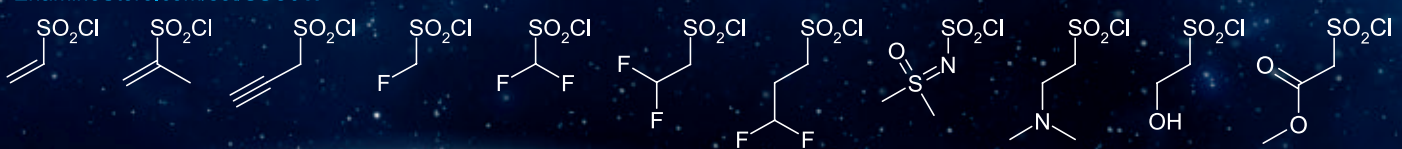

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GREEN CHEMISTRY

Electrosynthesis gives chemists more power

Organic chemists find using electric current as a reagent helps streamline reactions

STEPHEN K. RITTER, C&EN WASHINGTON

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Waldvogel's lab in Mainz, Germany, uses a variety of divided and undivided batch-type electrochemical cells (colored solutions added for visualization) for small-scale screening reactions and for prep-scale electrosynthesis.

When it comes to electrochemistry, the first thing that pops into mind probably isn't C–H activation or arene cross-coupling reactions. You might think of batteries and solar cells, or industrial processes such as electroplating and the electrolytic production of metals such as aluminum. Others might think of cyclic voltammetry, a technique used to study the chemical properties of compounds and reaction mechanisms.

But for plain old organic chemistry, like those arene cross-couplings, electrochemistry isn't common in research or used widely on a preparative scale. The century-old chlor-alkali electrolysis process to prepare chlorine and sodium hydroxide from sodium chloride solution is one exception. And emerging more recently have been clean energy electrocatalytic reactions such as splitting water to make hydrogen and reducing carbon dioxide to make simple hydrocarbons.

Today's chemists have been simply reluctant to adopt electrosynthesis, believing the technology is too cumbersome or expensive. Yet as a growing cadre of researchers is showing, the benefits of the technology can no longer be overlooked.

"Synthetic chemists have long viewed electrochemistry as an area where a few people do interesting reactions that are difficult for everyone else to repeat," says Kevin D. Moeller of Washington University in St. Louis. "That view is changing: The field is undergoing a dramatic uptick in popularity at the present, which for those of us who have been advancing the technique for a while now is really exciting."

"There is a real resurgence of electrosynthesis," adds Siegfried R. Waldvogel of Johannes Gutenberg University Mainz. "The invasion of more synthetically oriented scientists is propelling the area dramatically."

Synthetic organic reactions are fundamentally about adding and subtracting electrons to and from target molecules. Researchers achieve electron pushing typically through the power of an acid, base, or metal catalyst, accompanied by the activity of a cocatalyst or oxidizing and reducing agents to complete the circuit, so to speak, allowing the catalyst to be recycled.

In recent years, improvements in photocatalysis, in which light interacting with a catalyst helps drive the electron-transfer process, have further boosted organic synthesis. Electrosynthesis is offering a similar boost, except it's a pair of electrodes controlling electron flow in the reaction vessel instead of a lightbulb. Electrochemical synthesis shares some of the same perceived barriers to adoption as photocatalysis, but both approaches present the benefit for chemists to do more with less.

Electric current, when used as a surrogate reagent, offers researchers the ability to avoid toxic or dangerous oxidizing or reducing reagents, protecting groups, and catalysts typically used in organic synthesis. Moreover, reducing or eliminating heating and cooling of reaction vessels can cut energy consumption. Another plus is the ability to selectively target functional groups in a molecule during a reaction based on their different redox potentials, which is useful in diversifying intermediates and final products.

Those advantages play right into the hands of the modern synthetic organic chemist, who is faced with the challenge of creating increasingly complex molecules in a greener, more sustainable, safer, and more cost-effective manner over current reagent-based approaches.

Waldvogel's group, for example, in collaboration with researchers at Evonik Industries, last year created a metal-free, oxidant-free one-step electrochemical protocol for cross-coupling phenols to make symmetrical and nonsymmetrical biaryl diols (*Angew. Chem. Int. Ed.* 2016, DOI: 10.1002/anie.201604321 and 10.1002/anie.201605865). The researchers just expanded the approach to aniline-aniline cross-couplings to form 2,2´-diaminobiaryls (*Angew. Chem. Int. Ed.* 2017, DOI: 10.1002/anie.201612613).

Overall, the scalable "power-to-chemicals approach" is important for making specialty, value-added products, Waldvogel notes, including drug candidates, agrochemicals, flavors and fragrances, catalyst ligands, and molecules for materials science. And going beyond standard batch processes, Waldvogel's team is developing continuous electrochemical processes using microflow reactors, which can further increase efficiency and reduce waste.

"This stuff is extraordinary," Waldvogel exclaims. "These findings bring oxidative cross-coupling to the next level. Electrosynthesis represents a disruptive technology and will be a game changer for industry."

In another example, Jun-ichi Yoshida and coworkers at Kyoto University have

been helping advance electrosynthesis with a series of arene functionalization reactions. Yoshida's team carried out electrochemical oxidation of toluene derivatives to form benzyl cations that accumulate in solution, what Yoshida refers to as a "cation pool." Reactions with subsequently added nucleophiles give the desired benzylic C–H/aromatic C–H cross-coupling products. The Kyoto researchers have used this approach to make a variety of compounds, including a precursor of TP27, an inhibitor of protein tyrosine phosphatases. PTPases, as they are called, are regulators of cell growth and metabolism associated with conditions such as diabetes (*J. Am. Chem. Soc.* 2016, DOI: 10.1021/jacs.6b05273).

Taking another approach, Shannon S. Stahl's group at the University of Wisconsin, Madison, has been working toward developing more efficient electrochemical oxidation of biomass-derived alcohols. TEMPO (2,2,6,6-tetramethyl-1-piperidine *N*-oxyl) is an effective catalyst for such oxidations, but it requires running reaction cells at high electrode potentials. Stahl's group found that copper bipyridine and TEMPO work as cooperative partners for the two-electron oxidation of alcohols to make ketones and aldehydes. The dual electrocatalyst oxidations run at a fivefold faster rate and operate at an electrode potential a half-volt lower than that used for the TEMPO-only process (*Nature* 2016, DOI: 10.1038/nature18008).

"This is incredibly impactful research—the reemergence of electrochemistry deserves our attention," says Phil S. Baran of Scripps Research Institute California. Getting the attention of reluctant chemists isn't going to be easy, however, as Baran along with Evan J. Horn and Brandon R. Rosen in his group point out in a recent perspective article (*ACS Cent. Sci.* 2016, DOI: 10.1021/acscentsci.6b00091).

In their experience, the Scripps researchers find a number of electrosynthesis "fears" must be overcome. These include investing in equipment. The barrier to investment becomes higher, they note, when chemists discover that a standard instrument for preparative electrolysis doesn't exist and that many of the recent electrosynthesis success stories reported in the literature relied on home-built rather than commercially available equipment.

Adding to that fear, the Scripps researchers point out, is trying to understand the complex reaction setup, from the potentiostat to the endless number of variables encountered, such as deciding what type of reaction cell, electrode, or electrolyte to use for a given reaction. Plus, a common misconception is that only aqueous solvents can be used, when many organic solvents do work. Another misconception is that product separation is difficult.

Baran's group became involved with electrosynthesis out of necessity, he says, when his team was attempting to prepare the dimeric natural product diximaycin B. After extensive screening, the researchers couldn't find a chemical oxidizing reagent capable of forging the N–N bond needed to couple the two monomer units in the final reaction step. Only after exhaustive evaluations did they begin to consider an electrochemical oxidation.

Rosen, Baran, and their coworkers found a plausible method, assembled the needed equipment, and then dialed in the oxidation parameters to accomplish what no chemical reagent could. The achievement demonstrated "the power of electrochemistry in organic synthesis, particularly in complex settings that require exquisite chemoselectivity," Baran notes.

Baran's group now turns more often to electrosynthesis. For example, the researchers were looking for a practical chemical method for direct allylic C–H oxidations to make enone and allylic alcohol derivatives as intermediates for preparing terpene natural products. Typical approaches involve chromium or selenium reagents and palladium or rhodium catalysts, which are unsuitable in an industrial process, because of their toxicity or their cost.

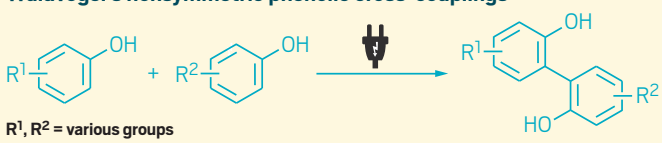
Horn, Rosen, Baran, and their colleagues, working in collaboration with chemists at Bristol-Myers Squibb, found an inexpensive *N*-hydroxyphthalimide catalyst that undergoes electrode oxidation to form an oxygen-centered radical that leads to the oxidation products. The researchers tested it by converting valencene to nootkatone, the major flavor compound in grapefruit. Process chemists subsequently used the approach to convert dehydroepiandrosterone derivatives to enones on a 100-g scale, eliminating the need for 80 g of a chromium reagent and the need to remove chromium-based contaminants from the product (*Nature* 2016, DOI: 10.1038/nature17431).

"Electrochemistry holds great promise for organic chemistry in terms of incredible efficiency and unique reactivity," Baran says. "But in order for it to really catch on, it will need to penetrate the most populated market of practicing organic chemists: Those in industry."

Leading the charge

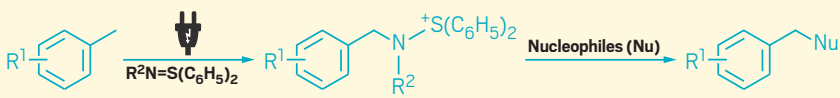
Multiple organic research groups are turning to electrosynthesis for a variety of reactions.

Waldvogel's nonsymmetric phenolic cross-couplings



R^1, R^2 = various groups

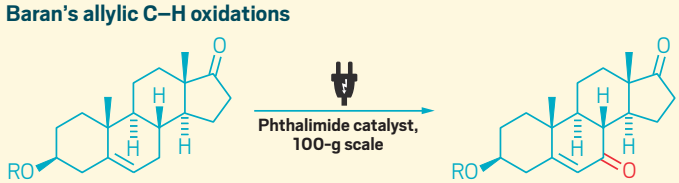
Yoshida's cation pool cross-couplings



Cation pool

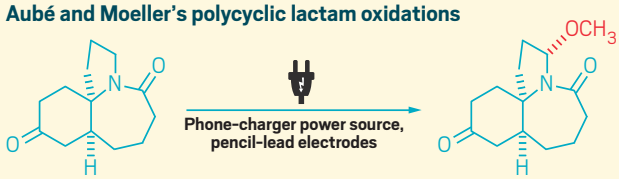
R^1 = various groups; R^2 = tosyl; Nu = heterocycles, unsaturated aliphatics

Baran's allylic C–H oxidations



R = H, $-COCH_3$

Aubé and Moeller's polycyclic lactam oxidations



That barrier also appears vulnerable to falling. "We are motivated by electrochemistry's ability to precisely control the flow of electrons in a redox process and its potential to access novel mechanisms," says Jeremy Starr, an associate research fellow at Pfizer whose group has been advocating organic electrosynthesis for several years. This power is amply illustrated, Starr notes, by the stories Baran and others are laying out, "which really capture the excitement of this field with some of the most inspiring examples of what currently can be done."

An especially important and perhaps underappreciated application for organic electrochemistry is in late-stage functionalization of drug lead compounds, Starr points out. His team has been using electrosynthesis to introduce oxygen or fluorine, or for making new C–C bonds, in small samples of complex molecules. At the other end of the spectrum, electrochemical oxidations, reductions, and cross-coupling reactions can offer synthetic and cost efficiencies for scale-up by sparing the use of stoichiometric quantities of reactants, he says.

"Like photoredox chemistry, I think the popularity of organic electrochemistry will grow as the perception of a high barrier to entry falls away, as inexpensive and easy-to-use power supplies and analytical tools become available, and as the relative ease of controlling and scaling the reactions becomes more broadly appreciated in the synthesis community," Starr observes.

Besides pushing to develop new electrochemically enabled reactions, the research groups leading the way are also pushing to develop instrumentation specifically for the organic synthesis community, in some cases collaborating with lab equipment companies. The goal for these new products is to offer what Baran calls "out-of-the-box" instrumentation, or what Waldvogel says is equipment "like a utility truck, not a high-end Ferrari." Waldvogel has already helped launch IKA's lab-scale continuous-flow electrosynthesis system, called Electrasyn Flow. Baran hints that a product codeveloped in his lab will be unveiled later this year.

For Washington University's Moeller, his group has been working for close to 30 years to make organic electrosynthesis more accessible. Moeller's team was one of the first to show that electrochemistry can be used to couple two nucleophilic reagents, opening up a new set of reaction pathways. The researchers have used these reactions along with electrochemical amide oxidations to synthesize a range of complex molecules. Many of these reactions can be driven by sunlight using solar cells or by other simple power sources, Moeller says, "providing evidence that anyone can do this."

To demonstrate, Moeller and his coworkers attached small photovoltaic cells normally used to power toy cars and boats or 6-V lantern batteries to the electrodes in their reaction flasks. Using these setups, they reproduced the yields of electrochemical reactions they originally ran with a conventional power supply. With Moeller's guidance, Jeffrey Aubé's group, then at the University of Kansas and now at the University of North Carolina, Chapel Hill, has shown how a repurposed cell phone charger can serve as a power supply and mechanical pencil leads can replace carbon electrodes. The researchers reported how that simplified equipment could be used for the C–H oxidation of polycyclic lactams in late-stage functionalizations (*Angew. Chem. Int. Ed.* 2015, DOI: 10.1002/anie.201504775).

"Over the period of many years, a series of dedicated scientists has explored electrochemical methods in ways that both illustrate their potential and define the experimental parameters needed to more fully capitalize on them," Moeller says. "Now with increasing pressure on the synthetic community to run more sustainable reactions, we have the opportunity to fully capitalize on this potential to enable a broad scope of synthetic transformations. No longer is electrochemistry the realm of specialists, and that change could not be more welcome." ■

Chemical firms exit 2016 with some bruises

Demand was strong for some specialties, but results showed the impact of slow growth and lower prices

MELODY M. BOMGARDNER, C&EN WEST COAST

U.S.-based chemical firms failed in their attempts to boost profits in 2016 in the face of an uneven and slow-growing global economy. The 19 chemical companies tracked by C&EN largely met earnings expectations for the final quarter. But for the full year, sales declined 5.3%, mainly because of lower raw material costs, while earnings fell 8.7%.

The picture looked rosier for the 17 firms that are not in the fertilizer business. Their combined earnings slipped by only 1.8%. And most specialty chemical makers, thanks to their value-added products, more than made up for lower materials costs to post significant earnings gains. In contrast, the fertilizer sellers Mosaic and CF Industries were hit hard by much lower selling prices and excess global supply.

The power of specialties to generate higher profits was particularly evident for companies that sell into consumer markets. In the fourth quarter, DuPont saw volume growth for sweeteners and probiotics aimed at the food industry and for performance materials used in automotive manufacturing. The firm also benefited from the popularity of its Solamet brand of metallization paste, used in solar cells.

Overall, DuPont's 2016 sales dipped slightly compared with 2015—not every specialty was in high demand—but earnings shot up by more than 27% to $2.9 billion. Chief Executive Officer Ed Breen credited the success to new product introductions as well as to the company's efforts to aggressively slim down in advance of its planned merger with Dow Chemical. In a conference call with analysts, he said DuPont trimmed 11% from its operating costs, including a 41% cut in corporate expenses.

The year was also a good one for DuPont's former performance chemicals businesses, Chemours. In its first full year of financial results, Chemours reported an earnings boost of 31% to $187 million, compared with the 2015 pro forma figures.

2016 financial review

Chemours CEO Mark Vergnano wrote in a note to investors that "2016 was about transformation; our five-point transformation plan delivered results on all fronts—cost reductions, portfolio rationalization, growth opportunities, focused capital investments, and cultural change." The company focused on lowering the cost of producing the white pigment titanium dioxide and growing its sales of Opteon, its line of low-greenhouse-gas-potential refrigerants.

Vergnano was also pleased about a recent agreement to settle thousands of lawsuits in Ohio and West Virginia over drinking water contaminated with perfluorooctanoic acid released from a former DuPont plant. DuPont and Chemours agreed to split the $670 million settlement, thus "addressing a key contingent liability" on Chemours's books, Vergnano wrote to shareholders.

Meanwhile, results at Dow were modestly higher on mixed performance in its diverse businesses. As at DuPont, consumer specialties blossomed: Sales were up 25% compared with 2015, and earnings more than doubled. Dow's purchase of all of Dow Corning amped up silicone sales to auto and consumer care markets. Plastics used in packaging continued their strong run. The firm also introduced ingredients for gluten-free products that were well received by the food industry.

But demand was lower for Dow's refining chemicals and performance monomers. Overall, Dow earned $4.2 billion for the year, up 4% from 2015.

For firms with portfolios tied more closely to basic chemicals, 2016 was not a great year. Huntsman Corp., Lyondell-

The year in chemicals

Specialties firms mainly had a good year, but basic chemicals and fertilizer companies struggled.

	SALES	EARNINGS[a]	CHANGE FROM 2015		PROFIT MARGIN[b]	
	$ MILLIONS		SALES	EARNINGS	2016	2015
Air Products	$9,051	$1,580	-1.6%	13.7%	17.5%	15.1%
Albemarle	2,677	483	-5.3	10.0	18.0	15.5
Ashland	4,978	415	-3.5	-11.7	8.3	9.1
Celanese	5,389	963	-5.0	5.0	17.9	16.2
CF Industries	3,685	109	-14.5	-87.8	3.0	20.8
Chemours	5,400	187	-5.5	30.8	3.5	2.5
Chemtura	1,616	111	-5.3	9.9	6.9	5.9
Dow Chemical	45,108	4,221	-3.4	4.1	9.4	8.7
DuPont	24,594	2,934	-2.1	27.5	11.9	9.2
Eastman Chemical	9,008	1,003	-6.6	-8.1	11.1	11.3
FMC Corp.	3,282	380	0.2	14.1	11.6	10.2
W.R. Grace	1,599	192	-1.8	8.5	12.0	10.9
Huntsman Corp.	9,657	377	-6.2	-23.4	3.9	4.8
LyondellBasell	29,183	3,865	-10.9	-20.0	13.2	14.8
Mosaic	7,163	298	-19.5	-70.2	4.2	11.2
NewMarket	2,049	243	-4.3	1.7	11.9	11.2
Praxair	10,534	1,576	-2.2	-6.0	15.0	15.6
Stepan	1,766	98	-0.6	24.1	5.5	4.4
Westlake Chemical	5,075	399	13.7	-38.2	7.9	14.5
TOTAL[c]	$181,814	$19,434	-5.3%	-8.7%	10.7%	11.1%

a After-tax earnings from continuing operations, excluding significant extraordinary and nonrecurring items. **b** After-tax earnings as a percentage of sales. **c** Percentages were calculated from combined sales and earnings.

Chemical top 10

Dow retook the top earner spot from LyondellBasell in 2016.

RANK 2016	SALES	$ MILLIONS	RANK 2015
1	Dow Chemical	$45,108	1
2	LyondellBasell	29,183	2
3	DuPont	24,594	3
4	Praxair	10,534	4
5	Huntsman Corp.	9,657	5
6	Air Products	9,051	7
7	Eastman Chemical	9,008	6
8	Mosaic	7,163	8
9	Chemours	5,400	9
10	Celanese	5,389	10

	EARNINGS	$ MILLIONS	RANK 2015
	Dow Chemical	$4,221	2
	LyondellBasell	3,865	1
	DuPont	2,934	3
	Air Products	1,580	5
	Praxair	1,576	4
	Eastman Chemical	1,003	6
	Celanese	963	8
	Albemarle	483	13
	Ashland	415	12
	Westlake Chemical	399	10

	PROFIT MARGIN	EARNINGS AS % OF SALES	RANK 2015
	Albemarle	18.0%	4
	Celanese	17.9	2
	Air Products	17.5	5
	Praxair	15.0	3
	LyondellBasell	13.2	6
	W.R. Grace	12.0	11
	DuPont	11.9	13
	NewMarket	11.9	10
	FMC Corp.	11.6	12
	Eastman Chemical	11.1	8

Note: Based on the companies listed on page 26.

Basell Industries, and Westlake Chemical all saw earnings shrink compared with the prior year. And for Eastman Chemical and Ashland, large specialties portfolios couldn't offset poor performance in commodity businesses.

Two Eastman specialties, Tritan copolyester and Saflex acoustic interlayers, benefited from strong demand, but its sales of fibers and lower-value copolymers fell. And lower raw material and energy costs decreased selling prices for its additives business, dampening results. Lower selling prices took a bite out of revenues at Huntsman's performance products and advanced materials businesses and affected sales of olefins at Westlake.

Mark Costa, Eastman's CEO, said the company is working to improve its mix of advanced materials to contain more high-margin products. The strategy will help the firm in 2017, according to Charles Neivert, chemicals analyst at the investment bank Cowen & Co. He noted in particular Eastman's success in developing and marketing high-performance tire resins and additives.

"Improved portfolio management should support additional earnings growth with lower volatility," Neivert wrote in a research note about the firm.

Ashland's specialty businesses had a strong year, yet overall earnings slipped 12% from 2015 as substantially lower selling prices dogged its butanediol operations. Its specialty ingredients division saw volumes increase 6% in the latter part of the year. In a note to investors, the company said, "Consumer specialties continued to drive growth across multiple end markets, notably hair care and oral care." Demand was also strong for Ashland's industrial specialties, mainly coating, adhesive, construction, and energy-related products.

In 2017, higher-cost petroleum plus an expansion in petrochemical manufacturing capacity could put pressure on profit margins in the industry, according to Laurence Alexander, chemicals analyst at the investment bank Jefferies. Still, he expects chemical firms to flex their muscles and raise prices as soon as they can.

"Our leading indicator for chemical sector pricing power is now the strongest since 2011, which supports chemical company aspirations to pass through higher input prices" in the second half of the year, Alexander wrote in a note to investors.

An increase in U.S. industrial manufacturing would strengthen pricing power by creating demand for larger quantities of raw materials supplied by the chemical industry. A second boost could come if manufacturing firms increase investments in equipment in addition to just churning out more products.

> "Our leading indicator for chemical sector pricing power is now the strongest since 2011."
>
> **—Laurence Alexander,** chemicals analyst, Jefferies

Both changes appear to be under way. In January, manufacturing activity expanded for a third straight month, according to the American Chemistry Council (ACC), the main trade group for U.S. chemical companies.

"Production was higher in several chemistry-intensive manufacturing industries, including food and beverages, appliances, construction supplies, machinery, electronics, semiconductors, petroleum refining, iron and steel products, paper, structural panels, printing, and furniture," ACC said in a weekly economics report.

Data on business investments are updated less frequently, but according to an index published by the U.S. Bureau of Economic Advisors, spending increased in both the third and fourth quarters of 2016. These measures and other indicators caused ACC's Chemical Activity Barometer to rise by 0.4% in February, which the group considers a "strong gain."

The chemical industry had embarked on a large round of deal-making when it looked as if economic growth would be slow for years. Now, it can look to postdeal restructuring as a way to capture more profit from a rebound in manufacturing.

Dow and DuPont continue their efforts to clear regulatory hurdles ahead of their historic merger, which is now expected to close some time in the first half of the year. In his conference call with analysts, DuPont's Breen reiterated his confidence that the deal will proceed and said the focus of regulators is mainly on the two firms' overlapping crop protection offerings.

But a flurry of other deals is also happening. Albemarle sold its surface treatment business to BASF in the fourth quarter of 2016. In January of this year, Air Products completed the sale of its performance materials division to Evonik Industries, making Air Products a pure-play industrial gas firm. And Air Products' main gas-selling rival, Praxair, will transform if a merger with Linde comes to fruition.

Ashland officially spun off its retail motor oil and service brand Valvoline into a publicly traded company last year. On Feb. 1, Chemtura's shareholders agreed to sell the company to Lanxess. Finally, Huntsman is working to spin off its TiO_2 business, to be called Venator, later this year. ■

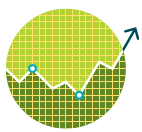
Pharmaceutical firms saw modest growth in 2016

Individual company results were mixed as sales of major products were beset by patent squabbles and expirations

ANN M. THAYER, C&EN HOUSTON

It was a rocky year for the pharmaceutical industry in 2016, made even more uneasy by infighting among companies.

Dynamics stemming from the U.S. presidential election, mergers, pricing, and global markets pushed and pulled drug company fortunes in many directions. Leading drugs experienced competitive and legal threats in what seemed a particularly litigious year filled with disputes among most major firms.



2016 financial review

Even so, the 18 companies that C&EN tracks fared well overall, with combined sales up about 5% and earnings increasing by nearly 6% from 2015. For traditional big pharma companies, it was a welcome change after four years of decline.

Factoring into this year's averages, however, were individual company results that ranged from significant double-digit gains to a like-sized drop. For Shire, a 78% jump in sales was a one-time event due to its acquisition of Baxalta in June. In most other cases, changes up or down centered on specific products.

Complicating the situation, the pharmaceutical industry found itself on a "patent cliff," a precipitous event occurring every three to four years when patent expirations add up. The roughly $50 billion per year in sales of products at risk in 2015 and 2016 were on the same order as that of the previous cliff, in 2012, according to data from the market research firm Evaluate.

The difference this time is the type of drugs losing patent protection and the potential blow to sales. In 2012, small-molecule drugs such as Lipitor fell off the cliff, and generic drug competitors cannibalized as much as 90% of sales. Now, several blockbuster biologics are losing protection to biosimilar versions, which are expected to cause less erosion than small-molecule generics.

Nevertheless, biosimilar competition is significant because the threatened biologics were seven of the top 10 drugs in 2016. Among those biologics is 2016's biggest seller, AbbVie's Humira. Sales of the anti-inflammatory rose 16% to $16 billion and accounted for more than 60% of the company's sales. By broadening the market for Humira, AbbVie has prevented the drug from showing its age.

AbbVie has also been trying to stave off impending competitors. In September, the Food & Drug Administration approved Amgen's biosimilar version, Amjevita, but not before AbbVie sued Amgen for patent infringement. Litigation is now under way, as is a separate dispute between Amgen and Roche about another biosimilar.

Amgen contends that Amjevita and other biosimilars it is developing will eventually contribute to growth, but for now the company must face competition to biologics it originated years ago. In 2016, Amgen's sales of the anti-inflammatory Enbrel and blood cell stimulants Epogen and Neupogen were all depressed by biosimilars.

Amgen's sales growth last year was just 6%, and that number may slip in the near future. "We will likely face headwinds in 2017 as declines in our mature brands will begin to offset volume growth from our more recently launched products," Amgen Chief Executive Officer Robert Bradway said on a conference call with analysts last month.

A similar trend is happening at Roche for its three leading products—the anticancer antibodies Rituxan, Avastin, and Herceptin—which enjoy more than $20 billion in combined annual sales. Competition from biosimilars and newer immuno-oncology therapies kept sales of the three products flat or only slightly up. Roche is betting on new drugs, including its recently launched immuno-oncology antibody Tecentriq, to help it regain ground.

The year in pharmaceuticals

A few standouts helped 2016 sales and earnings growth.

	SALES	EARNINGS[a]	CHANGE FROM 2015		PROFIT MARGIN[b]	
	$ MILLIONS		SALES	EARNINGS	2016	2015
AbbVie	$25,638	$7,904	12.2%	12.0%	30.8%	30.9%
Amgen	22,991	8,785	6.1	10.4	38.2	36.7
AstraZeneca	23,002	5,455	-6.9	1.2	23.7	21.8
Biogen	11,449	4,423	6.4	12.5	38.6	36.5
Bristol-Myers Squibb	19,427	4,750	17.3	40.6	24.5	20.4
Celgene	11,229	4,770	21.3	22.9	42.5	41.9
Eli Lilly & Co.	21,222	3,736	6.3	2.2	17.6	18.3
Gilead Sciences	30,390	15,713	-6.9	-18.1	51.7	58.7
GlaxoSmithKline	37,929	6,770	16.6	36.1	17.8	15.3
Johnson & Johnson	71,890	18,764	2.6	7.6	26.1	24.9
Merck & Co.	39,807	10,538	0.8	3.4	26.5	25.8
Novartis	48,518	11,314	-1.8	-6.0	23.3	24.4
Pfizer	52,824	14,761	8.1	7.3	27.9	28.2
Regeneron Pharmaceuticals	4,860	1,319	18.4	39.7	27.1	23.0
Roche	49,726	12,475	5.0	7.2	25.1	24.6
Sanofi	37,440	8,090	-0.7	-0.9	21.6	21.6
Shire	11,397	3,391	77.6	46.9	29.8	36.0
Vertex Pharmaceuticals	1,702	211	64.9	nm	12.4	def
TOTAL[c]	$521,441	$143,169	5.3%	5.6%	27.5%	27.4%

Note: European company results are converted at average annual 2016 exchange rates, except for AstraZeneca and Novartis, which report in U.S. dollars. **a** After-tax earnings from continuing operations, excluding significant extraordinary and nonrecurring items. **b** After-tax earnings as a percentage of sales. **c** Percentages were calculated from combined sales and earnings. **def** = deficit. **nm** = not meaningful.

Pharma top 10

Gilead trails J&J in earnings but is still tops in profitability.

RANK 2016	SALES		RANK 2015	EARNINGS		RANK 2015	PROFIT MARGIN		RANK 2015
		$ MILLIONS			$ MILLIONS			EARNINGS AS % OF SALES	
1	Johnson & Johnson	$71,890	1	Johnson & Johnson	$18,764	2	Gilead Sciences	51.7%	1
2	Pfizer	52,824	3	Gilead Sciences	15,713	1	Celgene	42.5	2
3	Roche	49,726	4	Pfizer	14,761	3	Biogen	38.6	4
4	Novartis	48,518	2	Roche	12,475	5	Amgen	38.2	3
5	Merck & Co.	39,807	6	Novartis	11,314	4	AbbVie	30.8	6
6	GlaxoSmithKline	37,929	7	Merck & Co.	10,538	6	Shire	29.8	5
7	Sanofi	37,440	5	Amgen	8,785	8	Pfizer	27.9	7
8	Gilead Sciences	30,390	8	Sanofi	8,090	7	Regeneron Pharmaceuticals	27.1	12
9	AbbVie	25,638	10	AbbVie	7,904	9	Merck & Co.	26.5	8
10	AstraZeneca	23,002	9	GlaxoSmithKline	6,770	10	Johnson & Johnson	26.1	9

Note: Based on the companies listed on page 28.

Likewise, Merck & Co. is seeing biosimilars start to erode the European market for the anti-inflammatory biologic Remicade. In the U.S., where Johnson & Johnson markets Remicade, FDA approved Pfizer's biosimilar version, Inflectra, in April. J&J's subsequent legal attempt to stop the launch failed.

Merck's sales were also hit by patent expirations on small-molecule drugs, including the antibiotic Cubicin, allergy drug Nasonex, and cholesterol-lowering therapy Zetia. AstraZeneca felt similar pressure from lost sales of the lipid-lowering drug Crestor. The firm reported a nearly 7% drop in sales. And at Novartis, sales dropped 2% as growth in new products only partially offset lost sales of its cancer drug Gleevec due to generic competition.

Along with cancer and inflammation, diabetes was another area where competition heated up. Sanofi's biggest product, the insulin analog Lantus, struggled against biosimilars and with patients switching to a newer product. As a result, sales of the drug fell more than 9% to about $6 billion. In August, FDA accepted Merck's application for approval of a biosimilar version of Lantus, prompting Sanofi to sue Merck for infringing 10 patents.

Sanofi and its partner Regeneron Pharmaceuticals were also on one end of a major patent battle, although not over biosimilars. Amgen sued the companies to prevent the sale of Praluent, a monoclonal antibody that competes with Amgen's cholesterol-lowering drug Repatha. The PCSK9 inhibitors have also attracted attention because of their high prices relative to competing drugs.

Similarly, Bristol-Myers Squibb and Ono Pharmaceuticals sued Merck over new PD-1 inhibitors for treating cancer. The companies settled earlier this year with a deal in which Merck will pay Bristol-Myers $625 million and royalties on sales of its drug Keytruda through 2026.

Despite the legal setback, Merck is generally seen as having taken the lead in the immuno-oncology drug area, especially after Bristol-Myers's drug Opdivo failed to perform as expected in some Phase III trials. Although Bristol-Myers's projections for 2017 are dampened, sales of Opdivo grew to $3.8 billion in 2016 from less than $1.0 billion the previous year.

Merck, meanwhile, won a lawsuit against Gilead Sciences about intellectual property rights to sofosbuvir. The compound is the active ingredient in Gilead's multi-billion-dollar blockbuster hepatitis C drugs Sovaldi and Harvoni. Gilead has been ordered to pay Merck $2.5 billion in damages, equal to 10% of the drugs' sales through August 2016. Gilead says it intends to appeal.

> The industry found itself on a "patent cliff," a precipitous event occurring every three to four years when patent expirations add up.

In 2016, Gilead saw sales of Sovaldi and Harvoni drop 35% and 24%, respectively, as successful treatment led to a decline in the relevant patient population. During the second half of the year, Gilead tried to fill the gap with a new product called Epclusa that can be used against all hepatitis C virus genotypes. Although lower in price than its predecessors, Epclusa still costs $75,000 per course of treatment. Sales of the drug reached $1.8 billion in 2016.

To keep a hold on its lead product, the multiple sclerosis drug Tecfidera, Biogen opted to pay the Danish biotech firm Forward Pharma a $1.3 billion licensing fee while the companies' patent interference dispute is under way. Sales of the drug reached almost $4.0 billion in 2016. Possible future royalty payments depend on whether Forward Pharma prevails in the dispute over rights to the drug's active ingredient, dimethyl fumarate.

The news in 2016 wasn't entirely bad, though, and a few companies boasted double-digit sales and earnings increases. Celgene continued to see strong growth for its cancer drug Revilmid, while Regeneron's gains were driven by sales of its eye drug Eylea. And Vertex Pharmaceuticals' sales of the cystic fibrosis drugs Orkambi and Kalydeco helped it turn the corner to profitability.

Drugmakers should also be heartened by Evaluate's prediction that 2017 will experience a slight drop in patent expirations that will last until about 2019. But the brakes are on sales of most of the current top 10, and to sustain growth, more new drugs will need to emerge. However, after two plentiful years, 2016 brought just 22 new drug approvals, a six-year low. ■

The venom of Australian funnel-web spiders is a rich source of insect-killing peptides.

AGRICULTURE

Spider venom: An insecticide whose time has come?

Bioinsecticide maker Vestaron says fruit and vegetable farmers are ready for its spider venom peptide

MELODY M. BOMGARDNER, C&EN WEST COAST

When it comes to solving difficult insect problems, it helps to consult an expert. For example, you could ask *Hadronyche versuta*, the Blue Mountains funnel-web spider. It has a few tried-and-true tools for killing: a funnel-shaped web to hide in, really large fangs, and a venom laced with the powerful insecticide versutoxin.

"It has a well-earned, fearsome reputation," says John Sorenson, chief executive officer of the biobased pesticide firm Vestaron. Like seemingly all things super venomous, the spider comes from Australia—specifically, the coastal range of New South Wales.

A farmer or gardener could travel to eastern Australia, gather up some *Hadronyche*, and milk them to obtain their insect-killing venom. But that's not very practical. So for years scientists have been working out how to make a pesticide based on, or inspired by, the spider's powerful weapon.

After successful registration with the Environmental Protection Agency in 2014, Vestaron is about to introduce its first product, which is based on a peptide in versutoxin. The insecticide, called Spear T, is effective against thrips, whiteflies, and spider mites in greenhouse settings. "Those three are the trifecta—the FBI most wanted—of greenhouse pests," Sorenson says.

Getting to launch has not been easy or quick. Vestaron was founded in 2001 with the more ominous-sounding name Venomix. That was before the time when pesticides based on biological, rather than synthetic, compounds were considered sexy.

Since then, major agrochemical companies have invested in biopesticides and acquired biobased chemical firms with the hope of providing more options to farmers. The marquee deal was Bayer's 2012 acquisition of AgraQuest for $425 million.

But even after a few decades of trying, convincing growers to adopt new pest control methods for their high-value fruit and vegetable crops is challenging. Early entrants were pricey and gave inconsistent results. To succeed, Vestaron will have to build a track record of efficacy, compete on price, and get visibility for its product in a marketplace crowded with bigger players.

"It's actually easier to develop a product than establish it on the market," warns Duane Ewing, an agricultural products consultant who was one of the cofounders of AgraQuest. "This is not for the fainthearted."

In 2016, the North American biopesticide market was worth $1.2 billion, only about 8% of total pesticide sales, according to Arun Ramesh, an analyst at the market research firm Frost & Sullivan. Bioinsecticides claimed 30% of that slice. Although biopesticide sales in general are growing by 11.5% annually, he says, bioinsecticides are stuck at 2% growth because of lingering farmer skepticism about their efficacy.

Even among biopesticides, Spear T is unusual. Most are used to kill fungal diseases, not insects. That's not surprising, because until now biopesticides have all come from soil bacteria, and bacterial chemical defenses are designed mainly to combat other microbes. Even the most famous biological insect killer, *Bacillus thuringiensis*, or Bt, is a protein made by a microbe.

And spider venom presented a web of challenges, Sorenson says. When scientists first attempted to identify and characterize venom peptides, they didn't have the

CREDIT: M. GRAY/AUSTRALIAN MUSEUM (TOP); WILLIAM BULLIMORE/AUSTRALIAN MUSEUM (BOTTOM)

necessary molecular biology tools. When that problem was solved, no one knew how to manufacture the peptides. And the peptides—large molecules the size of insulin—did not look like they would be bioavailable, except via spider bite.

Vestaron's active ingredient came out of research by Glenn King, a professor of chemistry and structural biology at the University of Queensland. King found a variety of disulfide-rich peptides in venom. Some are used for defense against other spiders or mammals, and others are tuned to kill insect prey. All of them work by disrupting ion channels of the victim's nervous system.

"The genius of Glenn's work is that he looked at the minor components that had broad insecticidal activity but not mammalian activity," Sorenson says. The peptide at the heart of Spear T is called GS-omega/kappa-Hxtx-Hv1a.

As an active ingredient, the peptide did not look very promising at first; its structure violated most of the rules said to define a good insecticide. It has a large molecular weight, is hydrophilic, and has many hydrogen donors. But surprisingly, tests showed that it kills some insects on contact.

The peptide blocks two ion channels in the insect nervous system—a voltage-gated calcium channel and a calcium-activated potassium channel. Both modes of action differ from the way Bt toxin and many other pesticides work. That means growers can use the peptide with other products to prevent the emergence of resistant insects. "It's a magnificent partner for rotation with other agricultural chemicals," Sorenson claims.

Vestaron scientists inserted the gene responsible for producing the peptide into yeast so it can be manufactured in large quantities via sugar fermentation. Last August, the company contracted Capua Bioservices to make its products in Italy.

Also in August, Vestaron's venture investors put an additional $18 million into the company. With the help of the funding, it is gearing up for distribution of Spear T and finalizing two follow-on products for release later this year and in 2018. The new versions will be combined with Bt to control caterpillars and the Colorado potato beetle.

Sorenson says the first Vestaron products will be price-competitive with "top-tier synthetic chemicals." But they can also play a different role than most synthetics because of their low toxicity to nonpest species, he says. After application, farm or greenhouse workers need wait only four hours rather than days to resume working. And Spear products can be applied right up until harvest.

Ewing, the consultant, sees more growth ahead for biological insect control. Even agchem companies wedded to synthetics are introducing products that mimic biological compounds to decrease damage to mammals and beneficial insects. "They're not like parathion where you spray and kill everything for 30 days," he says.

Vestaron, meanwhile, is screening synthetic mimics that share the insecticidal and toxicity characteristics of spider venom peptides. And it hopes to grow its market by inserting venom peptide genes into corn, cotton, and soybeans.

But for now, Sorenson is pleased to introduce a product he calls extraordinary. "It's the first peptide product of this kind ever to be commercialized," he says. ■

Vestaron at a glance

- **Founded:** 2001
- **Headquarters:** Kalamazoo, Mich.
- **Chief executive officer:** John Sorenson
- **Product:** Biobased insecticides
- **Employees:** 19
- **Funds raised:** $49 million
- **Investors:** Anterra Capital, Cultivan Sandbox Ventures, Pangaea Ventures, Open Prairie Ventures, Southwest Michigan First Ventures

Your guide to the ACS national meeting in San Francisco

C&EN's curated list of things to do, people to see, and science to learn

Must-see presenters

*** = Kavli speaker; ** = Plenary speaker**

Bradley Olsen*
Materials maestro, MIT

Jennifer Doudna*
Genome manipulator, UC Berkeley

Ann-Christine Albertsson**
Making sustainable polymeric materials, KTH Royal Institute of Technology

Jeffrey Linhardt**
Forget fingersticks. Verily Life Sciences researcher will present contact lenses that measure glucose in tears

Peter Green**
Cleaning up our energy act, National Renewable Energy Laboratory

Keith Watson**
Making industry–academia partnerships work for both sides, Dow Chemical

Natalie Franklin
Screening molecules without revealing structures protects collaborators' IP, Eli Lilly & Co.

Darren Lipomi
When bonded to gloves, his thin-film sensors can detect a hand forming American Sign Language letters, UC San Diego

Irene Groot
Imaging catalysts as they react, Leiden Institute of Chemistry

Charles Sykes
His rotor molecules perform computations, Tufts

Kathleen Page
Yet another reason to cut down on fructose. It affects the brain differently than glucose does, U of Southern California

Sechin Chang
USDA researcher describes milk protein casein's flame-retardant properties

Theresa Reineke
Polymer tailor, U of Minnesota

Christina Smolke
Programming yeast to produce medicinal opioids, Stanford

Michael Johnson
Probing the neurochemistry of "chemo brain," U of Kansas

Eranthie Weerapana
Her proteomic methods hunt down reactive cysteines, Boston College

Martin Burke
Replacing missing ion-transport proteins with "molecular prosthetics," UIUC

Carol Robinson
Mass spec maven, Oxford

Martin Thuo
Iowa State chemist recovers rare-earth metals from electronic waste, no dumpster diving involved. We think.

Wendy Young
Genentech VP will describe a potential lupus and rheumatoid arthritis treatment

CREDIT: SHUTTERSTOCK (ART); GOOGLE (MAP)

Checking out the neighborhood

Some attractions nearby and farther afield that you might want to see while you're in town.

1. Moscone Center: Your journey starts here.

2. Yerba Buena Gardens: This oasis in the city is also home to the Children's Creativity Museum. Find your inner child.

3. San Francisco Museum of Modern Art: In case the museum's 30,000 works of art aren't enough, you can roam Klee and Calder exhibitions too.

4. Union Square: In the heart of the city's shopping district, the central plaza is a great place to people watch.

5. Cable car turntable: Watch the famed cable cars change direction and then catch a ride to Chinatown.

6. W San Francisco (hotel)

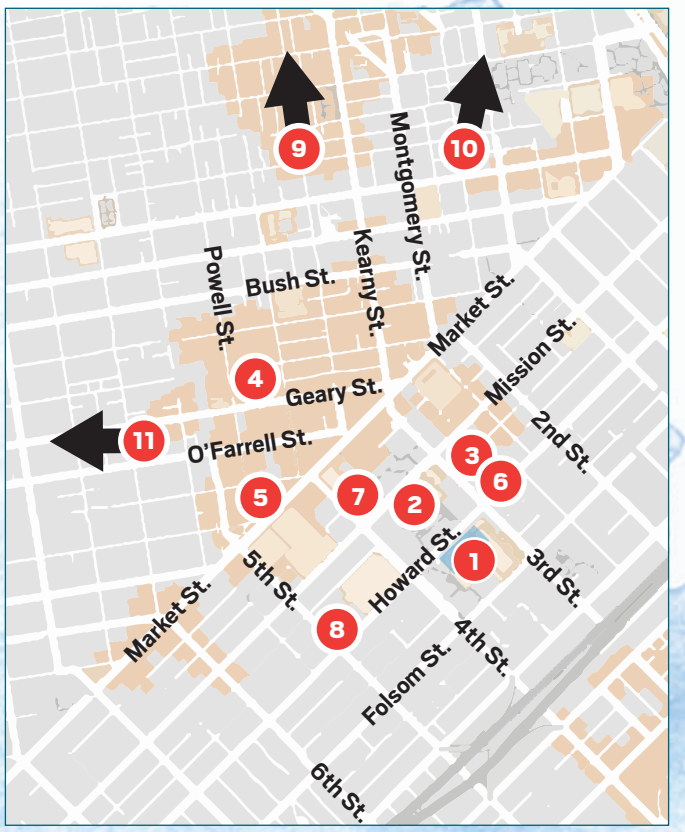
7. San Francisco Marriott Marquis (hotel)

8. InterContinental San Francisco (hotel)

9. Fisherman's Wharf: This waterfront neighborhood is home to Ghirardelli Square, a decommissioned World War II–era submarine, and a sea lion colony.

10. Exploratorium: If you stay till Thursday evening, you can check out this interactive science museum without competition from kids.

11. Golden Gate Park: With the California Academy of Sciences and its aquarium, the de Young art museum, and multiple gardens, there's something here for everyone.



More online

To find more details about the dates and times for these presenters and symposia—and even add them to your itinerary—visit **cenm.ag/sf2017.**

The pick of the program

Too bad there's no DVR for symposia. Here are some you should try to catch.

Chemistry of Korean Food & Beverages	Can't make it out for lunch? Get a vicarious kimchi fix instead.	Sunday all day
Chemical Forensics	Pull up a chair, amateur detectives. A session on chemical weapons kicks off the symposium.	Monday & Tuesday all day
Startup Road: BayBio and Beyond	Can you see them circling? This showcase of start-ups kicks off Sunday afternoon with the biotech version of "Shark Tank."	Sunday PM & Monday all day
Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities	This weeklong symposium runs the photochemistry gamut from photosynthesis to vision to excited-state dynamics.	Starts Sunday
Drug Discovery for ALS: Putting the Ice Bucket to Work	Come learn about recent advances in ALS research. We promise you won't get an ice bath.	Tuesday PM
What Have We Learned & Where Are We Going: Post-Settlement in the University of California	Hear about the progress that's been made in developing a safety culture on the UC campuses.	Wednesday all day
Hollyweird Chemistry	Producers and consultants for TV and film talk about getting the science right in popular entertainment.	Sunday PM & Monday all day

NOBEL PRIZE

C&EN talks with Fraser Stoddart, 2016 chemistry laureate

Northwestern professor discusses his legacy and hopes for scientists in China

JEAN-FRANÇOIS TREMBLAY, C&EN HONG KONG

Reporters interview Stoddart in Tianjin, China.

CREDIT: JEAN-FRANÇOIS TREMBLAY/C&EN

Tianjin, China, is as good a place as any to get a sense of how winning a Nobel Prize changes a person's life. Jean-Pierre Sauvage, Ben L. Feringa, and J. Fraser Stoddart co-earned the chemistry Nobel last November for their work on molecular machines, artificial molecules that can carry out tasks with a little jolt of energy. Stoddart led a team that created mechanically interlocked molecules, such as switchable rotaxanes, which can be used in molecular switches. C&EN recently caught up with Stoddart in China, where he's a visiting scholar at the School of Pharmaceutical Science & Technology at Tianjin University.

At an event held in Stoddart's honor, local reporters, students, and academics vied for his attention, either seeking his opinion, requesting an autograph, or wanting a selfie with the newly minted laureate.

On hand to celebrate Stoddart's success was his daughter Alison Stoddart and her three young children. "I've been trying to organize his inbox because it's been a bit overwhelming at times," said Alison, who is the chief editor of *Nature Reviews Materials*. "A lot of doors have opened for him since he received the Nobel, and I help him focus on what he really should respond to."

C&EN managed to ask Stoddart a few questions. The following, presented in a Q&A format, is partly the result of those interactions and partly from a presentation and discussion he had with local high school students in Tianjin about his personal and scientific life. Both the questions and answers have been edited for length and clarity.

How has life changed since winning the Nobel?

Northwestern University has put posters of me all over campus. When I enter the chemistry building, I have to push a door with a photo of me on it, which I don't actually notice anymore. I also have a personalized parking space.

Meanwhile, in Washington, D.C., the American Chemical Society headquarters building at one point set up a large banner with my name and face on it on their facade.

Aside from that, this new life has some negative and positive aspects that I try to manage. I've been trying to adjust to my new life as a minor celebrity. I have had the great privilege of pursuing my hobby—chemistry—in great facilities with good people for several decades, and now I have the opportunity to meet with presidents and prime ministers. [*Stoddart met with then-president Barack Obama at the White House in the U.S. in December, and he met with China's Prime Minister Li Keqiang in January.*]

What was it like to meet with Prime Minister Li?

Before the Nobel, the prime minister of Scotland, where I'm originally from, never asked to meet with me. But I talked with Premier Li last month as if he had all the time in the world.

We met in the Great Hall of the People [*a government building used for state dinners and ceremonies*]. Premier Li first asked me questions for about 12 minutes in front of everyone who was there. But he was not done with me. He sat next to me at the meal and didn't eat anything but instead grilled me with questions. He wanted to know what factors in my life led to my success and also what China could and should do to foster great people. China is looking for "best practices." The country is now supportive of what's called "blue sky" research [*curiosity-driven science*], and I really like this. Scotland, with a much smaller population than China, has generated three chemistry Nobelists out of about 170

Vitals

- **Hometown:** Edinburgh, Scotland
- **Positions:** professor of chemistry at Northwestern University; visiting professor of nanoscience and supramolecular chemistry in the School of Pharmaceutical Science & Technology at Tianjin University
- **Education:** B.Sc., University of Edinburgh, 1964; Ph.D., University of Edinburgh, 1966
- Hobbies**:** doing fundamental research, spending time with family (five grandchildren), keeping in touch with hundreds of former graduate students and postdocs worldwide, traveling, art collecting
- **Celebrity sighting:** In 2007, Queen Elizabeth II put a blade on my shoulder and made me a "Sir." Lord Chamberlain muttered: "I present to you Fraser Stoddart for services to chemistry and molecular nanotology." The Queen commented: "He got that wrong, didn't he?" She then correctly asked me about nanotechnology and whether it's about small things. I explained that nanoparticles are about 100,000 times smaller than a human hair. She replied that, indeed, that is "exceedingly small." That was the extent of our meeting.

ever awarded. So China has a lot of potential to foster great scientists.

You speak your mind on many topics. But, compared with Western countries, China restricts freedom of speech and opinion. Do you think China can really attract and develop great scientists?

Well, you can see that scientists in the U.S. are starting to be restricted in what they can say, so the difference is not as big as it used to be. Restrictions on freedom could be an impediment to creative research, but personally, I have never felt in China any restrictions on what I am allowed to say.

It's hard to write history as it's happening, but it's possible that China [*which is seeing thousands of scientists return home after training for years in the West*] is a country where creators are now moving to, a bit like Paris in prior centuries.

What can China do to foster great scientists?

I enjoyed going into a lab of my own and doing my own research. It's important to encourage creativity. You have to leave school wanting to be creative; you need a thirst for discovery.

Scientists should also be free of restrictive metrics on their performance. This is a problem in China, where there's a big emphasis on publishing many papers in science journals.

Will molecular machines built in the lab ever compete with those made by nature (such as kinesins that transport cargo in cells)?

Yes. It will happen in a few decades, and it will bring about a new Industrial Revolution. It will be mind-boggling. In much the same way as airplanes today exist comfortably alongside the birds and the bees and the bats, artificial molecular machines will exist seamlessly alongside nature's pumps and motors. Switchable rotaxanes have already been mounted on the surfaces of mesoporous silica nanoparticles to act as drug-release nanovalves in an attempt to develop controllable drug delivery systems for use in the fight against cancer.

What do you think your legacy in chemistry will be?

My legacy will not necessarily be my chemistry, which has been described in more than 1,000 publications—too many! It will be the more than 400 graduate students and postdoctoral fellows whom I have trained and mentored. Almost 100 of them have gone on to be professors in their own right in universities all around the world, while many more have gone into industry, government, finance, and publishing. It will be the young people I have trained who will be my legacy, particularly if they listen to my plea to tackle a big problem in science and not to continue doing "Stoddart chemistry" under any circumstances. Some heed my advice, and some ignore it. ■

Building pharmaceutical outsourcing partnerships

Three tales of creating new therapeutic molecules

Throughout the U.S. presidential election season and into the Trump presidency, the high cost of drugs has made for heated discussion. A popular topic for pundits is the amount drug companies spend on marketing compared to the generally smaller sum they spend on research.

Little attention, though, is paid to what it costs them to manufacture their products. That's in part because manufacturing is less glamorous than marketing and in part because it's a hard question to answer. Reports on the topic put manufacturing at anywhere from 15 to 50% of the overall cost of getting a drug to market.

What is clear is that molecules have to be built before they can be tested, approved, and sold. For small and start-up firms that don't have molecule-building assets of their own, contract service partners are essential to getting this job done.

In the pages that follow, C&EN presents stories of three small companies working on new drugs with outsourcing service partners. One of those drugs, Clovis Oncology's Rubraca, was approved by the Food & Drug Administration in December and is now selling for close to $14,000 per month.

People can argue over the price of the drug, but there is no disputing that Clovis owes some of its success to a pharmaceutical outsourcing partner.

In brief

- **Case study #1:** Clovis takes Lonza up on a dedicated plant for its cancer drug. P.37
- **Case study #2:** Immunomedics and Johnson Matthey connect for antibody–drug conjugates. P.42
- **Case study #3:** AMRI can do Nemus's cannabinoid chemistry. P.44

Clovis takes Lonza up on a dedicated plant for its cancer drug

The Swiss fine chemicals firm applies a biologics strategy to small-molecule manufacturing

RICK MULLIN, C&EN NEW YORK CITY

The Swiss fine chemicals firm Lonza is given credit for pioneering contract manufacturing of active pharmaceutical ingredients (APIs). Leading the way among its European cohort, Lonza pushed an industry in which APIs were made by drug companies in factories dedicated to a single product toward one in which they are produced under contract by chemical companies operating in versatile plants that can quickly switch capacity from one project to another.

Lonza's sprawling, Alps-nestled manufacturing site in Visp, Switzerland, has risen as a paragon of the multipurpose approach to manufacturing that now defines pharmaceutical outsourcing.

But it seems the company is now pointing in a new direction, roughly in reverse, as it begins building capacity dedicated to one product manufactured for one customer.

In October, Lonza announced plans to build a plant for a current client, Clovis Oncology, at which it will make the API for rucaparib, a drug approved last year to treat late-stage ovarian cancer. The new plant, which will go on-line in 2019, will consolidate disparate manufacturing processes and will include advanced automation, allowing for more-rapid release of materials than the batch-release process under which the product is currently made at Visp.

The partners will not discuss financial details or provide information on the volume of material being produced. But the drug, which won U.S. approval in December under the name Rubraca, is awaiting approval in Europe for the same indication. It's also in trials for broader application in ovarian cancer and in development for prostate cancer. Every indication is that volume will be higher by 2019.

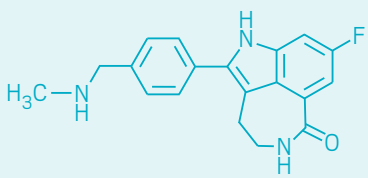
Lonza already operates dedicated plants for biologic APIs in Singapore and Portsmouth, N.H. The Clovis project will be its first such plant for a small molecule.

Patrick Mahaffy, chief executive officer of Clovis, says Lonza has been a dependable supplier ever since his company acquired rucaparib from Pfizer in 2011. But Clovis anticipates that increased demand for the product will tax the current approach of using multipurpose manufacturing assets at Visp.

"One issue is that part of the process requires being in a containment facility," Mahaffy says. "There is always a lot of competition to get in there." Above all, he says, Clovis needs Lonza to be able to respond to changes in demand that haven't had to be managed until recently.

"We went to Lonza and said, 'Let's see a proposal that addresses lead time and gets the cost of goods down,'" he recalls, "and they came back with a dedicated approach, which they have never done for a small molecule."

Rucaparib



- **Discovery**: A poly(ADP ribose) polymerase inhibitor first synthesized by scientists at Northern Institute for Cancer Research and the Medical School of Newcastle University, in partnership with the Pfizer subsidiary Agouron Pharmaceuticals
- **Development**: Clovis licensed the compound for development and commercialization worldwide in 2011
- **Approval**: Granted accelerated approval for use in cases of pretreated advanced ovarian cancer in December 2016
- **Status**: In clinical trials for broader treatment of ovarian cancer and development for treatment of prostate cancer

According to Christian Dowdeswell, Lonza's head of commercial development for chemical and microbial manufacturing, the request for a proposal came at a good time because Lonza was reviewing its approach to serving key customers. "We wanted to develop a better understanding of what our customers need and really start to tailor solutions to those needs," he says.

In Clovis's case, the needs were access to assets, security of supply, and production flexibility for variable but likely increasing demand. "We took a look and came up with this solution," Dowdeswell says. "The concept is a highly automated plant available to Clovis all year round with guaranteed access."

The plan calls for consolidating processes that are currently dispersed at the huge Visp site. "We have a wide breadth of high-potency and high-containment assets, and I think Clovis has touched most of those throughout the period of development," Dowdeswell says.

Engineering an integrated plant will lead to obvious efficiency improvements, he says, and the opportunity to introduce a higher level of automation will also allow "real-time release"—automated quality testing in the manufacturing line during production—of material that is currently released after finished batches are tested.

Converting from batch testing to real-time release can in some cases reduce production time from several months to a matter of weeks, Dowdeswell says.

Mahaffy agrees that automated testing will deliver key time and cost savings. "The use of real-time release will eliminate or greatly reduce the analytical testing necessary for each batch of drug substance and the associated quality review of that testing after the conclusion of processing," he says. "These costs are not a large component of the cost of goods, but they do contribute over time and large numbers of batches."

The more important benefit, he says, is inventory management. "Being able to move material quickly through the manufacturing facility without the need to hold material pending testing and release will allow more plant time to be dedicated to production. This could translate into more batches per year and

CREDIT: YANG H. KU/C&EN/SHUTTERSTOCK

correspondingly lower cost of goods."

Once production is completed, Mahaffy says, Clovis will be able to move the API to finished-dose manufacturing operations more quickly than from a batch-released operation, and ultimately to a product ready for sale. "This reduces the duration of time that we hold inventory in work-in-progress status," he says.

Dowdeswell concedes that building the plant for Clovis contradicts the "standard model" of multipurpose contract manufacturing that Lonza helped establish. "However, the multipurpose concept doesn't address some of our customers' fundamental needs in today's environment," he points out. "We took time to gain an understanding of what Clovis needed and to develop a concept for how to best address those needs and add value to our customer in ways that traditional business models cannot."

Lonza debuted the dedicated plant model for biologic drugs, most recently deploying it in a planned mammalian cell culture manufacturing facility for Sanofi in Visp. Lonza is now promoting it as an option for small molecules.

There are no guarantees in any pharmaceutical chemical manufacturing venture, and some question whether designing a plant for one customer's small-molecule drug makes sense.

Lonza will build a dedicated plant for a cancer drug at its expansive manufacturing site in Visp, Switzerland.

James Bruno, head of the consulting firm Chemical & Pharmaceutical Solutions, points out that the volumes of API found in new drugs are generally trending downward, meaning large amounts of capacity are typically not needed. And although FDA requirements for biologic drugs support a dedicated manufacturing model, the versatile multipurpose chemical plant may still be best for a large contract manufacturer such as Lonza, Bruno says.

There is little question, however, that engineering a plant to produce a single product will result in more efficient manufacturing, and Lonza and Clovis are optimistic that rucaparib will keep the new plant busy. It may also have a future beyond rucaparib.

"The plant is dedicated to this drug for now, but if the need emerges, it could be applied or modified for additional molecules as well," Mahaffy says. For the time being, however, Clovis is enthusiastic about the new approach to making rucaparib. "It was a great proposal from Lonza," Mahaffy says, "a really creative response." ■

CREDIT: LONZA

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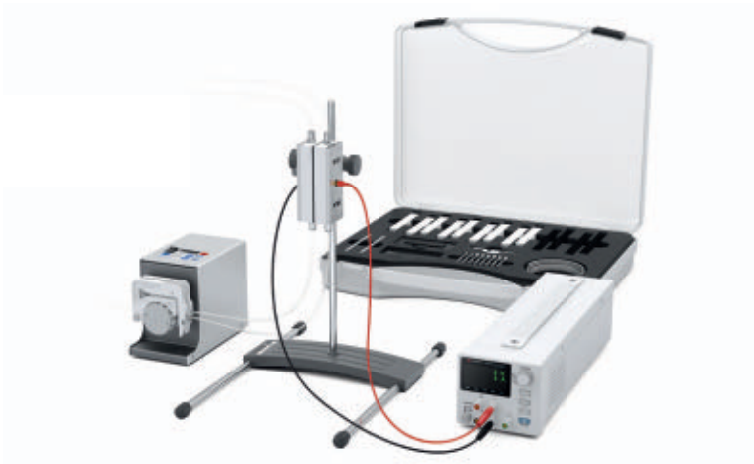

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Case study #2

Immunomedics and Johnson Matthey connect for ADCs

Special handling delivers drug and linker combo for creating tumor-targeting antibody-drug conjugate

ANN M. THAYER, C&EN HOUSTON

After 35 years of toil with few rewards, good things are finally coming to Immunomedics: It has a drug development deal worth up to $2 billion and a solid contract-manufacturing relationship. But the New Jersey-based firm also has an impatient shareholder that thinks it knows what's best for the company.

Although it got started in diagnostic imaging, Immunomedics has long tried to evolve into a drug company focused on targeted cancer therapies. It has built a pipeline of humanized monoclonal antibodies to be used alone as therapies or conjugated with radioactive isotopes, chemotherapeutics, cytokines, or cytotoxins.

The company's most advanced antibody-drug conjugate is sacituzumab govitecan, or IMMU-132. In the ADC, a long-chain chemical linker called CL2A connects SN-38, the active drug form of the chemotherapy agent irinotecan, to an antibody that targets the cell surface receptor TROP-2.

SN-38 is about 1,000 times as potent as irinotecan, but it can't be administered systemically because of its toxicity and poor solubility. The ADC is designed to deliver the chemotherapeutic payload directly to cancer cells while sparing healthy ones. So far, it seems to be working.

Immunomedics has reported good patient responses to IMMU-132 in Phase II clinical trials for several solid-tumor cancers. FDA has designated IMMU-132 as a breakthrough therapy for patients with triple-negative breast cancer who did not respond to other therapies and given it fast-track approval status for that indication as well as two forms of lung cancer. All this helped secure a licensing agreement worth up to $2 billion with ADC-specialist Seattle Genetics to finish development and commercialize IMMU-132.

Immunomedics got IMMU-132 to this point largely by itself. For early-stage work, "we manufactured the antibody, the linker plus the drug, and did the conjugation," says Cynthia Sullivan, Immunomedics's CEO. An outside manufacturer did the final formulation.

Because TROP-2 is present on a variety of solid tumors, Immunomedics moved to a "basket approach" for clinical trials, testing the drug for different indications simultaneously. "We are looking at about 13 different types of cancer," Sullivan says. The need for drug material has risen as a result of this approach, preparations for late-stage trials, and the fast-track approval status.

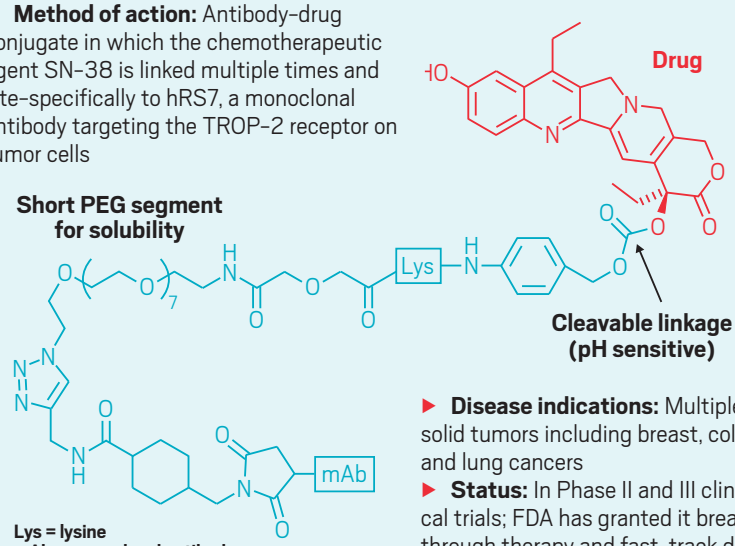
In 2013, Immunomedics started working with the contract manufacturer Johnson Matthey Fine Chemicals to scale up production. Johnson Matthey's custom pharma solutions unit in Devens, Mass., is tasked with making the linker and attaching it to SN-38. For now, Immunomedics still provides the antibody, but eventually Lonza will produce it at large scale in Singapore, Sullivan says. Italy's BSP Pharmaceuticals conjugates the pieces and completes the final formulation.

Though using multiple suppliers is logistically complicated, it is common in ADC development. "We haven't had any real issues in terms of supply," Sullivan says. As scale-up progresses, comparability testing of the original components made by Immunomedics and those from its contractors has been under way. Eventually all three suppliers must undergo their own preapproval inspections for Immunomedics to be able to market its product.

"Working with a supplier in the same time zone makes direct communication more streamlined and has helped us build a closer working relationship, but it was not a critical factor," Sullivan says about partnering with Johnson Matthey. "It was more important to identify a high-quality manufacturing organization with the right set of technology and expertise."

Sacituzumab govitecan (IMMU-132)

- **Active ingredient:** SN-38, the active metabolite of irinotecan
- **Method of action:** Antibody-drug conjugate in which the chemotherapeutic agent SN-38 is linked multiple times and site-specifically to hRS7, a monoclonal antibody targeting the TROP-2 receptor on tumor cells



Lys = lysine
mAb = monoclonal antibody
PEG = polyethylene glycol

- **Disease indications:** Multiple solid tumors including breast, colon, and lung cancers
- **Status:** In Phase II and III clinical trials; FDA has granted it breakthrough therapy and fast-track designations in different cancer types

Garrett Dilley, a senior director at Johnson Matthey, says the company already had the know-how and most of the equipment needed to support Immunomedics. Top on the list are production suites that can handle highly potent compounds such as SN-38. The firm was also familiar with developing and scaling up processes for linking small-molecule payloads to long-chain linkers and polymers for drug delivery applications.

Assembling the drug-linker combo presents some challenges, largely around protecting and derivatizing hydroxyl groups on the SN-38 molecule, says Serengulam V. Govindan, senior director for conjugation chemistry at Immunomedics. Most important, the CL2A linker is attached to SN-38's lactone ring to prevent the ring from opening and the molecule converting to an inactive carboxylate form. A short polyethylene glycol segment in CL2A helps solubilize the insoluble SN-38.

Given the complex nature of the drug-linker combo, a relatively large molecular weight "small molecule," according to Dilley, the project needs sophisticated analytical methods to understand parameters impacting quality, especially during scale-up.

Whereas Immunomedics was producing tens of grams of material, Johnson Matthey is making hundreds of grams and will reach kilograms. To prepare for full-scale manufacturing, Matthey is working to boost productivity. It is also using engineering techniques to increase efficiency in handling the molecule, given its potency, Dilley says.

This capability may be useful again because other ADCs in Immunomedics's pipeline—such as labetuzumab govitecan (IMMU-130), which is in Phase II trials for metastatic colorectal cancer—are based on the same drug-linker duo but conjugated to other antibodies.

The company's approach "differs from the current paradigm for making ADCs in the sense that the drug and the linker characteristics are quite different," Govindan says. Many ADCs in development use ultrastable linkers to avoid premature release of extremely toxic drugs before getting to a target. "We use a moderately potent drug" and instead conjugate more of it to the antibody, he says.

Immunomedics's chemistry, which involves a maleimide group on one end of the linker, allows for attaching up to eight drug molecules per antibody site-specifically at reduced interchain disulfides while avoiding the formation of dimers and aggregates. The pH-sensitive, cleavable linkage is moderately stable, with the potential to release SN-38 in the acidic tumor microenvironment and increase the drug's bioavailability. Together, these features allow for reduced toxicity, higher antibody doses, repeated therapy cycles, and a better therapeutic window, Immunomedics says.

Despite IMMU-132's success so far, not everyone is waiting patiently. Immunomedics's largest shareholder, the venture capital firm venBio, has been in a long and contentious battle with the company for control. It even opposes the recent deal with Seattle Genetics.

VenBio is concerned about the ability of Immunomedics's board and management to "realize the significant potential of IMMU-132." If the drug is approved, sales for four cancer indications could reach $7.5 billion per year by 2025, according to Jefferies stock analyst Matthew Andrews.

Immunomedics and venBio have tried to negotiate but are also suing each other. The decision over control came down to a shareholder vote held on March 3 that went in favor of venBio. As a result, it looks like a new plan may be in place for IMMU-132. ■

Case study #3

AMRI can do Nemus's cannabinoid chemistry

Service firm's government-approved assets are right for developing a drug based on psychoactive found in pot

MICHAEL MCCOY, C&EN NEW YORK CITY

Investors are hot on cannabinoids. Shares in GW Pharmaceuticals, marketer of the world's first plant-derived cannabinoid prescription drug, have more than tripled in the past year. The stock of Zynerba Pharmaceuticals, which is developing transdermal synthetic cannabinoids, has more than doubled.

In contrast, shares in Nemus Bioscience, the newest publicly traded cannabinoid company, have not caught on yet. And unlike its high-visibility competitors, which trade on the NASDAQ stock exchange, Costa Mesa, Calif.-based Nemus trades quietly on the less-prestigious over-the-counter market.

But Brian Murphy, Nemus's CEO, is biding his time. Murphy sees his firm as an up-and-coming player in second-generation cannabinoids. Nemus has been raising modest amounts of money from investors in preferred stock offerings. And importantly, it has signed up a respected contract research and manufacturing organization, Albany Molecular Research Inc. (AMRI), to develop and produce the active ingredient in its lead product.

Nemus got its start in 2012 after one of its founders, Cosmas Lykos, was approached by investors looking to capitalize on growing interest in cannabinoids. It went public two years later via a reverse stock merger with a trucking company called Load Guard Logistics.

"As is apropos for the area of cannabinoids, we are a little unconventional in how we were founded," Murphy acknowledges. Murphy himself has a pretty conventional background as chief medical officer for pharmaceutical firms including Valeant International, InterMune, and Roche.

Nemus's ace in the hole is a partnership with the University of Mississippi (UM), which since 1968 has held the sole federal contract to cultivate cannabis for research purposes. One of Nemus's scientific advisers is Mahmoud A. ElSohly, director of UM's marijuana project. "He literally wrote the book on cannabinoid chemistry," Murphy says.

In 2014, UM licensed Nemus the rights to tetrahydrocannabinol-valine-hemisuccinate (THC-VHS), a prodrug of THC, which is the main psychoactive component of the cannabis plant. Nemus renamed the compound NB1111 and is now developing it as a treatment for glaucoma. The company has several other cannabinoids in its pipeline as well.

Researchers have known since the 1970s that smoking marijuana reduces intraocular pressure in patients with glaucoma. "It's the first time in 20 years of drug discovery that I'm working with a drug I already know works before human trials have started," Murphy says.

But the smoking effect is short-lived, he notes, meaning patients have to stay almost constantly high for lasting glaucoma relief. THC eye drops would seem to be an option, but the molecule is lipid soluble and doesn't easily cross the cornea and get absorbed into the eye.

UM scientists discovered that attaching VHS to THC improves THC's water solubility. And once THC-VHS traverses the cornea, Murphy explains, esterases in the body cleave the amide-ester bond that links the molecule's two halves, freeing up THC.

UM followed up with rabbit tests showing that the effect of THC-VHS eye drops on intraocular pressure is better than that of THC alone or of existing treatments such as pilocarpine. However, researchers found no THC in the animals' circulatory system, indicating that a psychotropic effect was unlikely.

The next step for Nemus was finding a contract services firm that could further develop and produce THC-VHS to the standards that FDA demands before agreeing to human clinical trials. And because THC is considered a controlled substance, Nemus needed a partner with the right Drug Enforcement Agency (DEA) license.

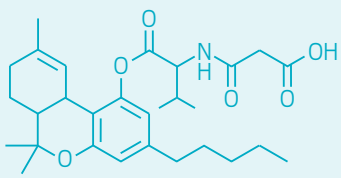
"Right away that filtered a lot of companies out of the mix," Murphy says. With the help of consultants who work with Nemus, he settled on AMRI.

AMRI, Murphy soon learned, isn't just licensed by the DEA to produce controlled substances. It has become something of an expert at cannabinoid chemistry. Pete Michels, a senior director and biocatalysis expert at AMRI, says the company has worked with close to a dozen partners on cannabinoid-based therapeutics.

As part of that push, Michels notes, the company is becoming a provider of unique cannabinoid molecules to the research community. Last year, for example, it licensed biosynthesis technology from Teewinot Life Sciences allowing it to produce the first commercial analytical standard for cannabichromenic acid, a nonpsychotropic cannabinoid being investigated as antiviral, antifungal, and anti-inflammatory.

Teewinot's technology uses biocatalysis to create cannabichromenic acid and other cannabinoids. Alternatively, cannabinoids including

NB1111



Tetrahydrocannabinol-valine-hemisuccinate

- **Active ingredient**: Tetrahydrocannabinol-valine-hemisuccinate
- **Discovery**: University of Mississippi
- **Development**: Nemus Bioscience
- **Disease indications**: Glaucoma; a related product, NB2111, is intended for managing chemotherapy-induced nausea and vomiting
- **Status**: Preparing for Pre-Investigational New Drug Application meeting with FDA

THC can be recovered through extraction from the cannabis plant.

But for Nemus's THC-VHS, AMRI is using a purely synthetic process that it developed in Rensselaer, N.Y., and scaled up for manufacturing at its Grafton, Wis., site. As with many natural products, AMRI and Nemus had some complex stereochemistry to solve, Michels says. AMRI also streamlined the synthesis with several process improvements, such as more-selective chemistry and the elimination of a chromatographic separation step.

Michels says AMRI and Nemus chose synthesis because it is reproducible, scalable, and unencumbered by the related cannabinoids that can come along with an extraction. "You want to ensure that no potentially psychoactive components are generated," he says. "This can be a significant advantage of synthesis versus botanical generation, which starts from a mix of compounds."

Others have noted that FDA and DEA are more comfortable with synthetic cannabinoids than with plant-derived ones. Tellingly, GW Pharmaceuticals' product Sativex, a multiple sclerosis treatment based on a mix of cannabinoids extracted from the cannabis plant, has yet to win approval in the U.S.

CREDIT: AMRI

In addition to controlled substances, AMRI's Rensselaer, N.Y., site handles scale-up of highly potent compounds.

Yet AMRI also uses extraction and fermentation in its broader pursuit of cannabinoid chemistry. "There are about 100 cannabinoids out there," Michels says. "Clearly, each of the three approaches can have advantages for specific molecules." By drawing on all three, he adds, AMRI is able to help customers investigate common cannabinoids such as THC and cannabichromenic acid, as well as lesser-known molecules.

Through acquisitions and internal growth, AMRI has become one of the largest U.S.-based providers of chemistry services to pharmaceutical companies. Its customers include some of the biggest names in the global drug industry. Nemus, on the other hand, is the smallest of start-ups.

But Christopher Conway, AMRI's senior vice president of discovery and development services, sees no disconnect. Serving small and virtual biotechs, he says, is core to what the company does. "Many of our largest commercial products started with a small biotech," he points out. "Part of our strategy is to create these 'sticky' customers."

And it doesn't hurt when that biotech firm is pursuing a high-profile area of chemistry like cannabinoids. "The market is very hot," Conway observes. "There's so much untapped potential that demand will continue to grow." ■

Join ACS in San Francisco!

3 Li 26 Fe Protecting Life's Elements

Meet the ACS Member Insurance Program Team

When you attend the 253rd American Chemical Society (ACS) National Meeting & Exposition and visit the ACS Member Insurance Program station, you can meet our knowledgeable team to learn about insurance plans available *exclusively* to ACS members. The exposition is being held **April 2 – 4, 2017** at the **San Francisco Moscone Center**.

Attention All Educators

This year, we're providing complimentary **Chemical Educators Legal Liability Consultations**. These sessions will contain important information on how our legal liability policy provides unique coverage, tailored specifically toward protecting educators. Visit **haysconsult.setmore.com** today to schedule your free 15-minute appointment.

For More Information

Visit **ACSplans.com/SanFrancisco** to learn more about our plans, including information on eligibility, features, limitations, costs, renewability, and exclusions, or to apply online. To speak directly with an insurance specialist, call **844.282.2438**.

ACSplans.com/SanFrancisco

ACS Insurance Plans

Member Insurance Program

Sponsored by the Board of Trustees
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COMMENT

Introducing fast and easy options to update bylaws

JAMES C. CARVER, CHAIR, ACS COMMITTEE ON CONSTITUTION & BYLAWS

For the past several years, the American Chemical Society Committee on Constitution & Bylaws (C&B) has worked diligently to demystify the process of amending bylaws. If you have not updated your bylaws recently, we urge you to do so because your bylaws are the rules and regulations about your officers and executive committee and how your unit conducts its business, including elections.

I have been a member of C&B since 2007 and have been honored to be its chair since 2014. I am happy to report that in late 2016, C&B modified the options to update bylaws for divisions, local sections, and international chemical sciences chapters, all known as units. These options are fast and easy, unless you prefer to customize your unit bylaws with special provisions.

In the past six years, C&B certified between 16 and 29 unit bylaws each year. Previously, the average number of bylaws certified per year was 13. The turnaround time from when we received proposed bylaws used to be three to four months; it now takes two to three weeks.

Options to update bylaws are available at www.acs.org/bulletin5; under **Unit BYLAWS,** click on **OPTIONS to AMEND your bylaws.** Choose whether you want to respond to the questions document, which gives default answers, or use the model bylaws, which are populated with the default answers from the questions document.

Officers of many of the units feel more comfortable starting with the model bylaws, wherein you have flexibility because you can modify the optional text, but the most common options are suggested. We recommend that you refer to the questions document for available options. Also, if there are any provisions in the unit's current bylaws that you would like to include in the proposed bylaws, let us know and we will check to see if the wording is consistent with the ACS governing documents.

If you wish, we will still do in-depth bylaw reviews for those units that want to fully customize their bylaws by using their existing bylaws as the basis for changes; required text from the model bylaws must be included. While this approach may require more work for the units and will likely take much longer for C&B to review, we do not want to prevent any unit from tailoring its bylaws as it sees fit. Our goal is to make sure the unit bylaws are internally consistent and consistent with the ACS governing documents and that the text is consistent with how the units wish to conduct their business.

It's now easier than ever to update your bylaws. The turnaround time from when we received proposed bylaws used to be three to four months; it now takes two to three weeks.

If you use either of the two easy options mentioned above and don't have any substantive changes other than optional text that is available, see "Next steps" below. If you'd like to discuss your proposed bylaws or any of the documents and/or options, C&B is available and happy to assist you.

Next steps: Send your proposed bylaws or the completed questions document to C&B. The committee will let you know when your bylaws are ready for a vote. Your members must vote on the proposed amendments in accordance with the unit's current bylaws, for which the certified version is available online as a PDF; contact C&B if you would like a Word document of your current bylaws.

After your members vote, the unit's chair or secretary will need to e-mail C&B the following required information so C&B can prepare its final report and certify the unit's bylaws: a) the date the announcement was sent to members to vote on the bylaw amendments; b) the results of the vote, including a statement that the vote passed in accordance with your current bylaws (for example, by two-thirds of the members voting); and c) a statement that all requirements for voting on the proposed bylaws have been followed in accordance with the current bylaws.

Depending on the number of bylaws in the queue for reviewing or certifying, we try to certify bylaws within two to three weeks from the date that your chair or secretary sends the vote results and other required information and documents.

Ten divisions have not updated their bylaws since 2010, and 89 local sections have not updated their bylaws since 2010; of these, 27 sections have bylaws certified in the 1970s. If your elections were conducted using electronic balloting and if this is not permitted by your bylaws, your elections might be invalid. It's now easier than ever to update your bylaws.

C&B is a standing committee of the ACS Council , for which only councilors may serve. If you are a councilor and interested in learning about and helping shape the governance of the society and giving input to bylaws, you should consider joining C&B, which meets on Sunday during ACS national meetings. Others are most welcome to attend the committee's open meetings, normally held Sunday afternoon during ACS national meetings.

For more information about C&B or help on your bylaws contact us at bylaws@acs.org or bpolansky@acs.org, or call (202) 872-4071.

Views expressed are those of the author and not necessarily those of C&EN or ACS.

CREDIT: GREMILLION PHOTOGRAPHY

253rd American Chemical Society National Meeting & Exposition

April 2-6, 2017 • San Francisco, CA

#acsSanFran • www.acs.org/sanfrancisco2017

ACS Chemistry for Life®

PRESIDENTIAL SYMPOSIA AND EVENTS

Photo: Peter Cutts Photography

Allison A. Campbell, Ph.D.
ACS President

SATURDAY, APRIL 1, 2017

12:00 PM - 4:00 PM
Presidential Outreach Event
Cosponsored by CCA
Exploratorium (Pier 15, The Embarcadero & Green St., San Francisco, CA)

SUNDAY, APRIL 2, 2017

9:00 AM - 5:00 PM
LGBT Graduate and Postdoctoral Student Chemistry Research Symposium
(Sponsored by PROF and Cosponsored by PRES, ANYL, BIOL, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, MPPG, ORGN, PHYS, PMSE, POLY & WCC)
Hotel Nikko San Francisco, Nikko Ballroom III (3rd Floor)

1:20 PM - 4:00 PM
Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal
(Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, ORGN & PROF)
San Francisco Marriott Marquis, Golden Gate A (B2 Level)

CHEMICAL SCIENCES ROUNDTABLE

SSURF Society for Science at User Research Facilities

MONDAY, APRIL 3, 2017

8:30 AM - NOON
Science for a Sustainable Energy Future: Energy Storage
(Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, ORGN PROF & SCHB, the Chemical Sciences Roundtable [CSR], and the Society for Science at User Research Facilities [SSURF])
Moscone Center, Room 133 (Moscone North, Hall E)

9:00 AM - 5:00 PM
LGBT Graduate and Postdoctoral Student Chemistry Research Symposium
(Sponsored PROF and Cosponsored PRES, ANYL, BIOL, CHED, CMA, COLL, COMP, CWD, ENVR, INOR, MEDI, MPPG, ORGN, PHYS, PMSE, POLY & WCC)
Hotel Nikko San Francisco, Nikko Ballroom III (3rd Floor)

1:30 PM - 4:30 PM
Science for a Sustainable Energy Future: Chemical & Biological Approaches to Energy Conversion
(Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, ORGN PROF & SCHB, the Chemical Sciences Roundtable [CSR], and the Society for Science at User Research Facilities [SSURF])
Moscone Center, Room 133 (Moscone North, Hall E)

SYMPOSIA RECOMMENDED BY THE ACS PRESIDENT

Best Practices in Selecting & Presenting Safety Training Content
(Sponsored by CHAS and Cosponsored by PRES & CCS)

Celebrating 90 years of the WCC: Reflections of Past Chairs
(Sponsored by WCC and Cosponsored by PRES & PROF)

Chemical Forensics
(Sponsored ANYL and Cosponsored by PRES & CHAL)

Chemists Leading the Charge: Chemists Using Business Acumen and Transformative Research to Address Societal Needs
(Sponsored by INOR and Cosponsored by PRES, BMGT, MPPG & PROF)

Communicating Science in the Twenty-First Century to Diversified Audiences
(Sponsored by CHED and Cosponsored by PRES & CWD)

Current Best Practices for Chemistry REU Programs
(Sponsored by CHED and Cosponsored by PRES)

Excellence in Graduate Polymer Research
(Sponsored POLY and Cosponsored by PRES, PROF, SOCED & YCC)

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten
(Sponsored by NUCL and Cosponsored by PRES & INOR)

GSSPC: Water Sustainability: Chemists in Pursuit of Clean Water
(Sponsored by CHED and Cosponsored by PRES & CEI)

PHYS Division Awards Symposium: Symposium in Honor of Barbara Finlayson-Pitts, Recipient of the Francis P. Garvan - John M. Olin Medal
(Sponsored by PHYS and Cosponsored by PRES)

Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators
(Sponsored by PROF and Cosponsored by PRES, BMGT & CHED)

Rising Star Award Symposium
(Sponsored by WCC and Cosponsored by PRES & BIOL)

Teaching, Researching and Community Building in the Global Chemical Enterprise
(Sponsored by IAC and Cosponsored by PRES, BMGT, ENVR, I&EC & PROF)

What Have We Learned & Where Are We Going: Post-Settlement in the University of California
(Sponsored by CHAS and Cosponsored by PRES & CCS)

San Francisco

CREDIT: SHUTTERSTOCK

ACS NATIONAL MEETING

253rd ACS National Meeting

San Francisco, April 2–6

"Advanced Materials, Technologies, Systems & Processes" will be the theme in San Francisco this April. Many notable symposia are scheduled, including "Communicating Science in the 21st Century to Diversified Audiences" and "Teaching, Researching & Community Building in the Global Chemical Enterprise."

ACS President Allison A. Campbell will host 29 technical divisions and six committees in original programming, including 1,100 half-day oral sessions and 144 poster sessions. More than 14,500 papers and nearly 5,700 posters will be presented.

Campbell will sponsor several presidential events. On Sunday and Monday, April 2–3, the two-day symposium "LGBT Graduate Student & Postdoctoral Scholar Chemistry Research" will include scientific talks by LGBT graduate students and postdoctoral researchers and a panel discussion on issues that affect LGBT students and postdocs. Sunday afternoon, "Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal" will assess the progress made in critical areas of chemistry since they were highlighted in a 1995 issue of the journal. On Monday, April 3, "Science for a Sustainable Energy Future" will focus on scientific advances in energy storage and chemical and biological approaches to energy conversion. Details on these and other presidential events can be found at www.acs.org/sanfran2017.

Many education-focused programs for high school teachers, undergraduate and graduate students, postdocs, and chemical professionals will be offered. A range of professional development courses will be available; ACS Professional Education Short Courses have a separate registration and fee. For job seekers and employers, the career fair will feature on-site interviews, one-on-one career assistance, and workshops.

The exposition will feature more than 250 companies showcasing services, instruments, books, and lab equipment in more than 400 booths.

The San Francisco area offers a mix of culture and natural beauty. Tour the infamous Alcatraz Federal Penitentiary, snack on dim sum in historic Chinatown, stroll through the popular Castro District, or explore natural history at the California Academy of Sciences. —ALEXANDRA TAYLOR

MEETING INFO ON THE WEB

www.acs.org/sanfran2017

REGISTRATION CATEGORY	FEES
MEMBERS	
ACS affiliate	$535
Postdoctoral member	535
Emeritus or retired member	270
50-year member	No fee
Unemployed member (Dues waiver required)	No fee
Precollege teacher	110
Graduate student	225
Undergraduate student	110
One-day registrant	270
NONMEMBERS	
Chemical scientist	$935
Postdoctoral scientist	935
Visitor: Nonchemical scientist or chemical technician	535
Precollege teacher	110
Graduate student	445
Undergraduate student	225
One-day registrant	535
Guest of registrant[a]	45
EXPOSITION-ONLY VISITORS	
Adult	$60
Student	30

a Registration is restricted to a spouse or family member of a registered attendee having no affiliation with the field of chemical science and who is not eligible to become an ACS member. Only one guest registration is allowed per registering attendee, and the guest registration must be completed and paid by the registering attendee at the time of original registration.

ACCOUNTS of chemical research

CELEBRATING 50 YEARS

Presidential Session — Holy Grails in Chemistry

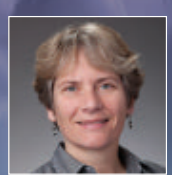
ACS Spring National Meeting & Exposition

APRIL 2, 2017 | 1:20 – 4:00 PM | MARRIOTT MARQUIS SAN FRANCISCO
780 MISSION STREET | SAN FRANCISCO, CA 94103

Join us as our distinguished presenters discuss what they identify as the most important challenges facing the chemistry research of today and for the future. This special session is part of the *Accounts of Chemical Research* Holy Grails of Chemistry Events and Special Issue, which celebrate the most influential challenges in the field.

SPEAKERS

Paul Alivisatos
University of California, Berkeley



Carolyn Bertozzi
Stanford University

Yi Cui
Stanford University

Hans-Joachim Freund
Fritz-Haber-Institut der Max-Planck-Gesellschaft

Melanie Sanford
University of Michigan

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ACS NATIONAL MEETING

General meeting information

Registration

All attendees, including speakers and poster presenters, must register for the meeting to participate in the technical sessions. Sponsored speakers should contact their symposium organizer or division program chair to clarify the terms of their invitation and to determine who will complete the speaker's registration. Attendees must display their badge at all times for admission to all official ACS sessions and events.

Early registration. Attendees in the U.S. who registered before Feb. 20 will receive their badge credentials by mail before the meeting. International registrants must pick up their badge credentials at ACS attendee registration (this includes Canada and Mexico).

Standard & on-site registration. Attendees who register after Feb. 20 must pick up their badge credentials on-site at attendee registration areas. On-site registration will be available at the Moscone Center, North Lobby; the Hilton SF Union Square, Ballroom Level, West Lounge; and the Grand Hyatt San Francisco, Theater Level. Cash transactions will not be available at the satellite registration areas. Only checks and credit cards can be used to make purchases at the satellite registration areas. ACS attendee registration will open at the Moscone Center, North Lobby, on Saturday, 3 to 6 PM; Sunday, 7:30 AM to 7:30 PM; Monday, 7:30 AM to 9 PM; Tuesday, 7:30 AM to 5 PM; Wednesday, 7:30 AM to 4 PM; and Thursday, 7:30 AM to 1 PM. The satellite registration areas will follow the same schedule but are subject to change depending on the activity at the location.

Satellite registration & on-site program pickup. Printed copies of the on-site program book will no longer be available for free. In support of ACS's sustainability efforts, we encourage the use of the ACS San Francisco mobile app and digital program for quick access to the meeting's full technical program, maps, and search features.

Prefer a printed on-site program? The on-site program book will now be available for a $20 fee. The author index will be included in the printed program booklet. Purchase your copy during the registration process or visit the locations listed below. Limited quantities will be available. Replacement copies also cost $20. Cash transactions will not be permitted at the satellite registration areas. Only credit cards or checks can be used to make purchases at the satellite registration areas. Printed programs can be picked up or purchased at the following locations:

- Moscone Center, North Lobby
- Hilton SF Union Square, Ballroom Level, West Lounge
- Grand Hyatt San Francisco, Theater Level

Learn about ACS national meeting sustainability efforts at www.acs.org/greenermeetings. Questions? Contact nationalmeetings@acs.org.

Travel

TRANSPORTATION DISCOUNTS. ACS has negotiated special travel discounts with the following partners. To get the best rates and avoid service fees, it is recommended to make reservations online (except for Amtrak).

AIRLINES:
Delta
delta.com/meeting; (800) 328-1111
Discount code: NMPBR

United Airlines
united.com; (800) 426-1122
Discount code: ZXMC508834

TRAIN:
Amtrak
(800) 872-7245
Discount code: X90C-958 (phone reservations only)

CAR RENTAL:
Avis
avis.com; (800) 331-1600
Discount code: B923099

Hertz
hertz.com; (800) 654-2240
Discount code: 02UZ0016

AIRPORT GROUND TRANSPORTATION. San Francisco International Airport is located 13 miles south of downtown San Francisco.

Public transportation. San Francisco has a comprehensive public transportation system that includes the Bay Area Rapid Transit (BART) system, Caltrain commuter rail, and SamTrans public bus service. For more information, please visit bit.ly/2jueoyY.

Taxi services. Taxis depart from the designated taxi zones located at the roadway center islands, on the arrivals and baggage claim level. Fares range from $46.16–$66.16. A $2.00 exit surcharge is included in all San Francisco taxicab meter fares for rides originating from San Francisco International Airport.

TRAVELING TO MEETING VENUES. The Moscone Center is located at 747 Howard St.

ACS shuttle. Complimentary shuttle service will be provided between the Moscone Center and official ACS hotels, with the exception of hotels within walking distance.

Parking. There is no parking provided at the Moscone Center for attendees or exhibitors. Nearby parking garages are listed on the Moscone Center website.

Events & activities

A variety of organizers will host special events during the meeting. Event participation is open to all interested registrants. **All**

ACS badge reprint policy

First badge reprint: No charge; upon proper identification and confirmation of registration payment, a duplicate badge is issued.
Second badge reprint: Attendee completes a duplicate badge request, shows identification, and pays a charge of $25 (cash/credit card), and a duplicate badge is issued.
Third badge reprint: Attendee completes a duplicate badge request, shows identification, and pays a charge of $50 (cash/credit card), and a duplicate badge is issued.
Beyond third badge reprint: Attendee completes a duplicate badge request, shows identification, and pays a charge of $100 (cash/credit card), and a duplicate badge is issued.

nonticketed events require a visible registration badge for entry.

Tickets are sold on a first-come, first-served basis. Ticket sales will close at 6 PM the evening before the event. Some event organizers may offer a limited number of tickets for sale at the door of the event. The deadline for cancellation and refund requests was March 6.

Locations and times are subject to change. To learn more about these events and to buy tickets or register, visit www.acs.org/sanfran2017.

▶ Friday, March 31

CHAS Laboratory Waste Management
8 AM to 5 PM, Moscone Center, Room 120

CHAS Laboratory Safety Workshop
8 AM to 5 PM, Moscone Center, Room 121

▶ Saturday, April 1

CHAS Cannabis Extraction & Analysis Workshop
8 AM to 5 PM, Moscone Center, Room 120

CHAS How To Be a More Effective Chemical Hygiene Officer
8 AM to 5 PM, Moscone Center, Room 121

CHAS Using ACS Lab Safety Resources in the Classroom
8 AM to 5 PM, Moscone Center, Room 124

CHAS Reactive Chemical Management for Laboratories & Pilot Plants
8 AM to 5 PM, Moscone Center, Room 125

COACHing Strong Women in the Art of Strategic Persuasion
8 AM to 5 PM, SF Marriott Union Square, Sutter 1

COACh Upping the Game: Refresher Workshop for Past COACh Alums
8 AM to 5 PM, SF Marriott Union Square, Sutter 2

COACh Reception
5 to 7 PM, SF Marriott Union Square, Russian Hill

FOR UP-TO-DATE EVENT LISTINGS, VISIT
www.acs.org/sanfran2017

▶ Sunday, April 2

Undergraduate Hospitality Center
8 AM to 5 PM, SF Marriott Marquis, Salon 7

Career Pathways Workshops
8 AM to 5:30 PM, W San Francisco, Great Room 2

Career Pathways I
8 AM to 5:30 PM, W San Francisco, Workroom 1

Career Pathways II
8 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8 AM to 5:30 PM, W San Francisco, Workroom 3

Making the Most of Your First National Meeting
8:30 to 9:15 AM, SF Marriott Marquis, Salon 7

Graduate School Reality Check, Part 1: Getting In
10 to 11:30 AM, SF Marriott Marquis, Golden Gate Ballroom B

Graduate & Postdoc Focus Group
10 AM to noon, Moscone Center, 2nd floor, Area 2

Chem Demo Exchange: Household Chemicals
11 AM to 12:30 PM, Moscone Center, Hall A

Graduate School Reality Check, Part II: You're In—Now What?
11:30 AM to 12:45 PM, SF Marriott Marquis, Golden Gate Ballroom B

ACS Board Luncheon & Meeting
Noon to 1 PM, Moscone Center, Gateway Ballroom 103/104

CHED High School/College Interface Luncheon/SE-01/$45
Noon to 1 PM, SF Marriott Marquis, Salon 7

POLY Board Meeting
Noon to 1 PM, Moscone Center, Room 132

Developing Communication Strategies
Noon to 5:30 PM, Park Central San Francisco, Commonwealth

BIOT Lunch Seminars
12:30 to 2 PM, InterContinental San Francisco, InterContinental B

CTA Awards Luncheon/SE-02/$45
1 to 3 PM, Hilton SF Union Square, Continental Parlor 3

Networking Social with Graduate School Recruiters
1 to 5 PM, Moscone Center, Hall A

Networking 101
1:30 to 3 PM, SF Marriott Marquis, Golden Gate Ballroom A

Graduate & Postdoc Focus Group
2 to 4 PM, Moscone Center, 2nd Floor, Area 2

Two-Year to Four-Year College Transfer Survival
2:30 to 3:30 PM, SF Marriott Marquis, Golden Gate Ballroom B

Advanced Materials, Technologies, Systems & Processes Plenary Session
3 to 6 PM, Moscone Center, Gateway Ballroom 103 & 104

SciBabe: Chemistry Blogging
4 to 5:30 PM, SF Marriott Marquis, Golden Gate Ballroom A

On-site program book no longer free

Copies of the on-site program book will be available for $20. In response to numerous requests, the author index will be included in the printed program booklet. Satellite registration and on-site program purchase/pickup will be located at the Moscone Center, Hilton Union Square, and Grand Hyatt San Francisco. Credit cards, debit cards, and checks will be accepted at these locations.

In support of ACS's sustainability efforts, we encourage our meeting attendees to download the ACS San Francisco mobile application or access the ACS San Francisco digital meeting program with author index in early April. These digital options will provide quick access to the full technical program, along with special features so you can easily build your schedule.

MEETING INFO ON THE WEB

Registration, housing, technical programming, special events, participating exhibitors, and other meeting details are available at www.acs.org/sanfran2017.

IAC Networking Globally: Helping Chemistry Students Find Success in Careers and Study Abroad/SE-03/no charge
4 to 5:30 PM, Hilton SF Union Square, Yosemite C

Faculty and Postdoc Afternoon Coffee Break
4 to 6 PM, Hotel Nikko San Francisco, Monterey I

Diversity Reception
5 to 7 PM, Hilton SF Union Square, Yosemite A & B

AGFD Poster Session Reception
5 to 7 PM, Moscone Center, West Hall

University of Wisconsin, Madison, Alumni & Friends Social Hour
5 to 7 PM, Park Central San Francisco, Concordia Park

University of California, San Diego, Alumni & Friends Social Hour
5 to 7 PM, SF Marriott Marquis, Salon 1

University of Illinois, Urbana-Champaign, Alumni & Friends Reception
5 to 8 PM, InterContinental San Francisco, Sutter

District I Councilor Caucus
5:30 to 7 PM, Hilton SF Union Square, Union Square 1 & 2

CHED Social Reception
5:30 to 7 PM, Moscone Center, Room 130

COLL Social Hour/Poster Session
5:30 to 8 PM, Moscone Center, Halls B/C

INOR Poster Session
5:30 to 7:30 PM, Moscone Center, Hall D

ORGN Poster Session
5:30 to 7:30 PM, Moscone Center, West Hall

C&EN DIGITAL MEETING PROGRAM AVAILABLE AT

cenm.ag/sanfran2017

Joint Research Corporation Petroleum Research Fund Reception in Honor of the Awardee for Research at an Undergraduate Institution
5:30 to 7:30 PM, Hilton SF Union Square, Golden Gate 4 & 5

International Welcome Reception/SE-04/no charge
5:30 to 7:30 PM, Hilton SF Union Square, Grand Ballroom A

District II Councilor Caucus
6 to 7 PM, Hilton SF Union Square, Union Square 3 & 4

District III Councilor Caucus
6 to 7 PM, Hilton SF Union Square, Union Square 5 & 6

District IV Councilor Caucus
6 to 7 PM, Hilton SF Union Square, Union Square 15 & 16

District V Councilor Caucus
6 to 7 PM, Hilton SF Union Square, Union Square 17 & 18

District VI Councilor Caucus
6 to 7 PM, Hilton SF Union Square, Union Square 19 & 20

SCHB Entrepreneurs' Poster Session
6 to 8 PM, Moscone Center, Halls B/C

University of Washington Alumni & Friends Reception/SE-27/$5.00
6 to 8 PM, W San Francisco, Great Room 1

Attendee Welcome Reception
6 to 8:30 PM, Moscone Center, Halls B/C

CINF Welcoming Reception and Poster Session
6:30 to 8:30 PM, Park Central San Francisco, Franciscan I & II

PROF General Posters
6:30 to 8:30 PM, Moscone Center, Halls B/C

Student Chapter Awards Ceremony
7 to 8:30 PM, Hilton SF Union Square, Grand Ballroom B

ANYL Poster Session
7 to 9 PM, Moscone Center, West Hall

MEDI General Posters
7 to 9 PM, Moscone Center, West Hall

CHED Poster Session
7 to 9 PM, Moscone Center, Hall D

BIOL Poster Session
7 to 9 PM, Moscone Center, West Hall

FLUO Poster Session
8 to 10 PM, Moscone Center, Hall D

Undergraduate Social
8:30 to 11 PM, Hilton SF Union Square, Continental 1–6

▶ Monday, April 3

Women in the Chemical Enterprise Breakfast/SE-05/$40 (regular)/SE-06/$20 (undergraduate)
7:30 to 9 AM, Hilton SF Union Square, Imperial B

YCC Fun Run/SE-07/$30 (regular)/SE-08/$15 (undergraduate)
8 to 10 AM, Moscone Center, outside West Lobby

Engaging Colleagues in Dialogue
8 AM to noon, Park Central San Francisco, Commonwealth

Undergraduate Hospitality Center
8 AM to 5 PM, SF Marriott Marquis, Salon 7

Career Pathways I
8 AM to 5:30 PM, W San Francisco, Workroom 1

Career Pathways II
8 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8 AM to 5:30 PM, W San Francisco, Workroom 3

Improving Scientific Communications
9 to 10:15 AM, SF Marriott Marquis, Golden Gate Ballroom B

ACS Exposition
9 AM to 5 PM, Moscone Center, Halls B/C

Women Chemists of Color Networking/SE-09/no charge
10:30 AM to noon, Hilton SF Union Square, Yosemite C

CRC Handbook Discussion Forum
11:30 AM to 3 PM, Moscone Center, Room 134

Committee on Minority Affairs Luncheon/SE-10/$50 (regular)/SE-11/$25 (undergraduate)

11:30 AM to 1:30 PM, Hilton SF Union Square, Grand Ballroom A

CHAL Drug & Power Luncheon/SE-12/$40
Noon to 1:30 PM, Mourad, 140 New Montgomery St.

Undergraduate Research Poster Session
Noon to 2 PM, Moscone Center, Hall D

BIOT Lunch Seminars
12:30 to 2 PM, InterContinental San Francisco, InterContinental B

Leading Change
1 to 5 PM, Park Central San Francisco, Commonwealth

Women Chemists Committee Open Meeting and 'Just Cocktails' Reception
4 to 5 PM, Hotel Nikko San Francisco, Nikko Ballroom II

The Kavli Foundation Emerging Leader in Chemistry Lecture
4 to 5:10 PM, Moscone Center, Gateway Ballroom 103/104

The Fred Kavli Innovations in Chemistry Lecture
5:15 to 6:30 PM, Moscone Center, Gateway Ballroom 103/104

CHAL Reception
6 to 8 PM, Jillian's, 175 Fourth St.

CACS Dinner Banquet/SE-13/$37
6:30 to 9 PM, Far East Café, 631 Grant Ave.

ACS Graduate & Postdoctoral Scholars Reception/SE-14/no charge
7 to 8:30 PM, Moscone Center, Room 134

UC Berkeley Dept of Chemistry Alumni & Friends Reception
7 to 8:30 PM, InterContinental San Francisco, Grand Ballroom C

Sci-Mix Interdivisional Poster Session/ (drink ticket with registration)
8 to 10 PM, Moscone Center, Hall D

Event participation is open to all interested registrants. Some events require a ticket or registration to participate. Payment and **SE-##** ticket requirements, when applicable, are indicated in the event list. All nonticketed events require a visible registration badge for entry. View an updated listing of events and activities at www.acs.org/sanfran2017.

▶ Tuesday, April 4

University of Minnesota Alumni & Friends Breakfast/SE-16/$5.00
7:30 to 9:30 AM, Moscone Center, Room 2000

Senior Chemists Breakfast/SE-15/$20
7:30 to 9:30 AM, Hilton SF Union Square, Grand Ballroom A

Coaching & Feedback
8 AM to noon, Park Central San Francisco, Commonwealth

Career Pathways I
8 AM to 5:30 PM, W San Francisco, Workroom 1

Career Pathways II
8 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8 AM to 5:30 PM, W San Francisco, Workroom 3

NSF Graduate School Fellowships
9 to 9:45 AM, SF Marriott Marquis, Golden Gate Ballroom A

ACS Exposition
9 AM to 5 PM, Moscone Center, Halls B/C

Women Chemists Committee/Eli Lilly Travel Award Poster Session
11 AM to noon, Hilton SF Union Square, Grand Ballroom A

Alpha Chi Sigma Fraternity Luncheon
11:45 AM to 1:30 PM, John's Grill, 63 Ellis St.

CINF Division Luncheon/SE-20/$30
Noon to 1:30 PM, Park Central San Francisco, Franciscan I

COLL Luncheon/SE-19/$45
Noon to 1:30 PM, W San Francisco, Great Room 1

WCC Luncheon/SE-17/$50 (regular)/SE-18/$25 (undergraduate)
Noon to 1:30 PM, Hilton SF Union Square, Grand Ballroom A

Chemistry & the Environment Film Series
Noon to 2 PM, SF Marriott Marquis, Golden Gate Ballroom B

BIOT Lunch Seminars
12:30 to 2 PM, InterContinental San Francisco, InterContinental B

Leading without Authority
1 to 5 PM, Park Central San Francisco, Commonwealth

Local Section Officers, Outreach Coordinator & Speakers Reception
3:30 to 5:30 PM, Hilton SF Union Square, Continental Ballroom 4

Division Officers & Councilors Caucus
4 to 5:30 PM, Moscone Center, Room 132

ANYL Dinner/SE-21/$25 (regular)/SE-22/$15 (undergraduate)
5 to 7:30 PM, Hilton SF Union Square, Golden Gate 2

Henry Hill & Lou Sacco Award Reception
5 to 7 PM, Hotel Nikko San Francisco, Nikko Ballroom III

UCLA Research Showcase
5 to 7 PM, Moscone Center, Room 135


Lombard Street

CREDIT: SHUTTERSTOCK

Sacramento Region Meet & Greet Reception
5 to 7 PM, W San Francisco, Great Room 1

INOR Poster Session
5:30 to 7:30 PM, Moscone Center, Hall D

ORGN Poster Session
5:30 to 7:30 PM, Moscone Center, Hall D

Moissi Kick-Off Reception
5:30 to 7:30 PM, Hotel Nikko San Francisco, Bay View

Division Officers & Councilors Caucus Reception
5:30 to 6:30 PM, Moscone Center, Room 133

POLY/PMSE Joint Poster Session
6 to 8 PM, Moscone Center, Hall A

BIOT Poster Session
6 to 8 PM, Moscone Center, West Hall

COMP Poster Session
6 to 8 PM, Moscone Center, West Hall

ENVR Division Reception/SE-23/$20
6 to 8 PM, ThirstyBear Brewing Co., 661 Howard St.

NUCL Social Hour
6 to 8 PM, Moscone Center, Room 130

CATL Poster Session
6 to 8 PM, Moscone Center, Hall D

ENFL Awards Dinner/SE-24/$60
6:30 to 9 PM, Le Colonial, 20 Cosmo Pl.

CELL Awards Banquet/SE-25/$65
6:30 to 10 PM, The Chart House, Pier 39

ACS National Awards Banquet Ceremony & General Meeting/SE-26/$130
6:30 to 10 PM, SF Marriott Marquis, Salons 8/9

BIOL Poster Session
7 to 9 PM, Moscone Center, West Hall

▶ Wednesday, April 5

Career Pathways I
8 AM to 5:30 PM, W San Francisco, Workroom 1

Career Pathways II
8 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8 AM to 5:30 PM, W San Francisco, Workroom 3

Chemical Forensics International Technical Working Group
8:30 AM to 5 PM, Hotel Union Square, Continental Ballroom 4

BIOT Lunch Seminars
12:30 to 2 PM, InterContinental San Francisco, InterContinental B

POLY/PMSE Lecture & Awards Reception
5:30 to 8 PM, Moscone Center, Room 134

ENVR Poster Session
6 to 8 PM, Moscone Center, Hall D

GEOC Poster Session
6 to 8 PM, Moscone Center, Hall D

I&EC Poster Session
6 to 8 PM, Moscone Center, Hall D

PHYS Poster Session
7 to 9 PM, Moscone Center, Hall D

NUCL Poster Session
7 to 9 PM, Moscone Center, Hall D

MEDI & ORGN General Poster Social
7 to 11 PM, Moscone Center, West Hall

JACS

JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

Spotlight on Advanced Materials Technologies, Systems, and Processes

ACS Spring National Meeting & Exposition

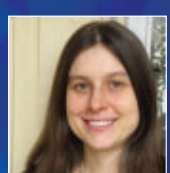
APRIL 2, 2017 | 8:30 AM - 11:30 AM | ESPLANADE BALLROOM 301
MOSCONE CENTER, 747 HOWARD ST. | SAN FRANCISCO, CA 94103

Join us for this symposium that highlights advances by *JACS* contributors in research areas that align with the theme of *Advanced Materials Technologies, Systems and Processes*, from energy to health and beyond.

SPEAKERS

Tanja Weil
Max Plank Institute for Polymer Research, Germany

Shelley Minteer
University of Utah



Marta Cerruti
McGill University, Canada

Peidong Yang
UC Berkeley

Nanfeng Zheng
Xiamen University, China

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Exposition

SEE WHAT'S NEW INSIDE THE EXPOSITION. Visit the ACS National Exposition at the Moscone Center, Halls B/C, from Sunday, April 2, through Tuesday, April 4. The show hours will be Sunday, 6 to 8:30 PM, and Monday and Tuesday, 9 AM to 5 PM.

Companies will showcase services, instruments, books, computer hardware, scientific software, and an array of chromatographic, lab, and safety equipment. Technical personnel will give demonstrations, answer questions, and discuss your needs and interests.

Visit the revamped ACS Career Fair where you'll meet recruiters from top companies such as KAUST, Merck, Gilead, Georgia Pacific, and many more. Create an online profile and upload your résumé to our database, where recruiters can schedule in-person interviews with you. While at the Career Fair, network with potential employers and drop off your résumé, attend Career Pathways workshops, and meet with ACS Career Consultants.

Also, join us at the ACS booth in the middle of the exposition floor, where ACS staff members will present the many benefits, services, products, and merchandise offered by ACS.

Online exposition. The online exposition is a component within the exhibitor directory that enables attendees to view videos, press releases, brochures, and flyers of participating exhibitors. Access the online exposition at www.acs.org/sanfran2017 to learn more about exhibiting companies and download product information that meets your needs.

Free exhibitor workshops. Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the Moscone Center. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity. Register at www.acs.org/sanfran2017 to reserve your seat.

Presentations & special events. Join us on Sunday from 6 to 8:30 PM for the attendee welcome reception. Take an afternoon break on Tuesday from 3 to 5 PM and visit the exhibitors before the exposition closes. Access the mobile app, play a game with participating exhibitors, and win special prizes!

Internet & technology. Get free internet access and leave messages for one another at the meeting mail terminals located throughout the meeting. Enjoy free Wi-Fi service at designated areas in the Moscone Center.

Admission requirements & expo-only registration. Exposition admission is complimentary for all national meeting registrants; however, you are required to wear your badge. Individuals who want to visit the exhibits without registering for the technical component of the national meeting can obtain an expo-only badge for $60. Students with school identification can obtain an expo-only badge for $30. Registration can be handled online or in person at ACS attendee registration at the Moscone Center, North Lobby, and at our satellite registration areas at the Hilton San Francisco Union Square and Grand Hyatt San Francisco.

Exhibitor workshops

▶ Sunday, April 2

McGraw-Hill Education Learning Technologies Workshop. *Sponsor:* McGraw-Hill Education, 3:30 to 6 PM, Moscone Center, Room 250. Join McGraw-Hill Education to learn about the technology available to provide a unique learning experience for every student. Learn about ALEKS, Connect, SmartBook, and more!

▶ Monday, April 3

Teaching Laboratory Safety in the Undergraduate Chemistry Curriculum. *Sponsor:* Flinn Scientific Inc., 9:30 AM to noon, Moscone Center, Room 250. Many faculty and lab managers at undergraduate institutions often find it difficult to incorporate laboratory safety throughout their courses. Join us as we discuss how to integrate Flinn Scientific's new, engaging online student laboratory safety course and other valuable safety resources into your curriculum, and learn how these resources can be used to build a positive safety culture in your department and school.

Solutions for Innovation. *Sponsor:* JEOL USA, Inc., 9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 2. Ambient ionization mass spectrometry, scanning electron microscopy, and NMR structure: Learn how the latest innovations from JEOL integrate to enhance your science.

Advancing Material Science Research through Spectroscopy. *Sponsor:* ThermoFisher Scientific, 9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 1. New materials present new analytical challenges. Like many labs today, you need to stay ahead of the curve. This workshop will show you how FTIR and Raman spectroscopy can be applied in your lab, from the discovery of new materials to solving production problems and ensuring product quality. An industry expert will guide you through the latest trends and techniques to solve your toughest challenges.

How To Make LC Method Development and Peptide Mapping Simpler; Tackle Interferences with Advanced Triple Quadrupole Technology. *Sponsor:* ThermoFisher Scientific, 12:30 to 3 PM, Moscone Center, Hall B, Exhibitor Workshop Room 1.

Part I: How to Make LC Method Development and Peptide Mapping Simpler. Why should method development and peptide mapping be a challenge? Come and see how the latest developments in UHPLC afford method transfer from any LC with higher levels of reproducibility as well as resolution, and how when it comes to peptide mapping, we haven't just revolutionized one part of your workflow, we have revolutionized them all!

Part II: Tackle Interferences with Advanced Triple Quadrupole Technology.

Getting Real with Organic Chemistry. *Sponsor:* CAS, 12:30 to 3 PM, Moscone Center, Hall B, Exhibitor Workshop Room 3. Students are often left wondering, "Why should I care? How does this apply to me and my future career?" Professors are tasked with trying to connect the real world with the concepts taught in textbooks. Come hear how Chemistry Class Advantage™, a new digital learning solution from CAS, will help you teach the relevance of organic chemistry, as well as bridge the gap between memorization and conceptual understanding.

What Can NMR Do for the Chemist? Introduction to Experiments Beyond 1D Proton and Carbon Spectra. *Sponsor:* Bruker, 12:30 to 3 PM, Moscone Center, Room 250. With the modern NMR hardware and software available today, many of the experiments that used to be considered complicated and unnecessary are now quite routine and extremely beneficial to the chemist. This workshop will present an introduction to the alphabet soup of NMR experiments and explain what they are, what information can be obtained from them, and when to use one over another.

Topics will include the following:

- 2-D experiments commonly used for structure verification and elucidation such as COSY, TOCSY, HSQC, and HMBC.
- Examination of NMR active nuclei that might be of interest to the inorganic chemist and important things to consider when running these experiments.
- Brief introduction to magic angle spinning (HR-MAS and MAS) methods.
- A quick look into the possibilities of triple resonance biomolecular NMR.

Wiley Workshop: Technology in the Modern General Chemistry Classroom. *Sponsor:* Wiley, 12:30 to 3 PM, Moscone Center, Hall B, Exhibitor Workshop Room 2. Please join Wiley as we explore the trends and challenges of teaching general chemistry utilizing technology. Collaborate with your peers on what's working well and what's needed to improve student engagement and performance in this course. Share your feedback on a forthcoming, digital general chemistry project from Jason Kautz of the University of Nebraska, Lincoln. Lunch will be served.

Seamless Integration of 2-D to 3-D SAR to Guide Multi-Parameter Optimization. *Sponsor:* Optibrium Ltd., 3:30 to 6 PM, Moscone Center, Hall B, Exhibitor Workshop Room 1. This hands-on workshop in collaboration with BioSolveIT will explore how the combination of 2-D structure activity relationships (SAR) with 3-D structure-based design can be used to guide the optimisation of novel, high-quality compounds. Practical examples will be illustrated using both Optibrium's StarDrop and BioSolveIT's SeeSAR software.

McGraw-Hill Education Learing Technologies Workshop. *Sponsor:* McGraw-Hill Education, 3:30 to 6 PM, Moscone Center, Room 250. Join McGraw-Hill Education to learn about the technology available to provide a unique learning experience for every student. Learn about ALEKS, Connect, SmartBook, and more!

▶ Tuesday, April 4

Mass Spec Inlet Versatility to Maximize Productivity. *Sponsor:* Advion, 9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 1. With the daily need to analyze liquids, solids, vapor-phase compounds, and even air-sensitive samples, the ability to change sample inlets is indispensable. Learn how a single instrument can be adapted to each of these sample requirements and rapidly changed to accommodate back-to-back assays. Listen to users in the field speak about the innovative sample inlets that have cut down on prep and streamlined their everyday workflow.

Innovative HPLC Solutions to Increase Efficiency and Productivity in the Lab. *Sponsor:* Agilent Technologies, 9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 2. This workshop will focus on two topics: increasing productivity of biotherapeutic characterization in drug development and developing rapid HPLC methods with sufficient resolution and speed. Details of using novel HPLC instrumentation, software, and column chemistries will be discussed with time for Q&A with Agilent application scientists.

Engaging Millennials in the Classroom: A Panel Discussion with Dr. Neil Garg. *Sponsor:* Top Hat, 11 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 3. With millennials demanding a more engaging learning experience, higher education instructors have had to evolve their teaching methods. Through this lively panel discussion moderated by Dr. Neil Garg, hear about tips and tricks that experts in the field are using to foster active learning both inside and outside the classroom.

Raman inVia Qontor and LiveTracking. *Sponsor:* Renishaw, 12:30 to 3 PM, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 3. inVia Qontor: Accurate Raman imaging of rough samples and/or those with complex surface topographies is now even faster with the new Renishaw ultra-fast Centrus detector. RA802 is a dedicated pharmaceutical analyser for imaging tablets to determine API size and distribution metrics from coatings and particles.

Advancing HPLC and GC Separations. *Sponsor:* Agilent Technologies, 12:30 to 3 PM, Moscone Center, Hall B, Exhibitor Workshop Room 2. QbD solutions for analytical method development in HPLC: Real-world data will be presented demonstrating unique ways to overcome analytical challenges. Plus, Agilent will provide an introduction to modern 2-D HPLC for multiple sample types. See the latest developments on this exciting workflow that you can implement today. Also witness a new era in gas chromatography, the Intuvo 9000 GC. Resolve your search for more ions by discovering the advantages of Agilent's GCMS solutions.

Vibrational Spectroscopy for Pharmaceutical Applications. *Sponsor:* Bruker, 12:30 to 3 PM, Moscone Center, Hall B, Exhibitor Workshop Room 1. The latest advances in the FTIR and Raman instrumentation and applications will be reviewed in this seminar, with a thorough discussion of the following topics:

- Contaminations in pharmaceutical products.
- Reverse engineering.
- Structural changes in proteins.
- Maximization of protein stability.
- Chemical imaging of biological tissues.

Examples of applications will include analysis of protein secondary structure, protein melting point determination, bacteria recognition, and analysis of tablets.

The seminar will include a live demonstration of the new Bruker FTIR microscope and a hands-on session. Attendees are encouraged to bring samples of interest for analysis during the hands-on session.

▶ Wednesday, April 5

Electrochemistry 101: Experiments for Use in Undergraduate Labs. *Sponsor*: Gamry Instruments, 9:30 AM to noon, Moscone Center, Room 250. Gamry Instruments has developed a complete laboratory course in electrochemistry for undergraduate facilities. The course includes experiments designed to engage students and provide them the opportunity to explore various disciplines in chemistry, such as analyte characterization, aqueous sample testing, digital simulations, electrosynthesis, sensors, batteries, and corrosion. The complete educational bundle includes the instrument, teaching and student manuals with eleven separate experiments, as well as all cells and electrodes needed to complete a semester course for 20 students. This workshop will be an introduction to all aspects of the course material via the performance of select experiments.

Structure-Based Drug Design and Ligand Modification. *Sponsor*: Chemical Computing Group, 3:30 to 6 PM, Moscone Center, Room 250. The course covers MOE applications for interactive, structure-based design. Examples include active site visualization, protein-ligand contact analysis, and ligand modification/optimization in the receptor pocket. Conformational searching and analysis of the ligand to assess ligand flexibility will be discussed. A protocol for aligning and superposing protein complexes in the context of protein selectivity will be studied.

EXHIBITORS

The following list of exhibitors, as of Feb. 11, is the property of the American Chemical Society. Any unauthorized use of this list, or any part thereof, either directly or indirectly, is strictly prohibited.

Visit the Online ACS National Exposition at www.acs.org/sanfran2017 to download the updated exhibitor list and access product information.

101, 375 South End Avenue, Apt. 9G, New York, NY, United States 10280, 917-587-7883, Internet: www.101edu.co *101 builds subject-specific classroom engagement tools that promote active learning in college STEM courses. Our first product for chemistry courses, Chem101, was piloted with 2000 students across 8 schools in Fall 2016 including Carnegie Mellon, Columbia University, and the University of Cincinnati.* **1530**

abcr GmbH, Im Schlehert 10, Karlsruhe, Germany 76187, +49 721 950 61101, fax: +49 721 950 6133, Internet: www.abcr.de *With abcr, you have access to over 260,000 products from the organic, organometallic and inorganic specialty chemicals area.*
- *R&D services: custom synthesis, research projects*
- *Production: research, syntheses, scale-up, pilot and commercial plant in our production facilities*
- *Semi bulk / bulk business*
- *Catalogue business: procurement and sales of specialty chemicals* **1718**

Accela ChemBio Co. Ltd., 9883 Pacific Heights Blvd., Suite H, San Diego, CA, United States 92121, 858-699-3322, fax: 858-769-6322 or 858-876-1948, e-mail: info@accelachem.com, Internet: www.accelachem.com *Accela ChemBio focus on design, synthesis, manufacture R&D chemicals and pharmaceutical intermediates for worldwide scientific research institutions and industrial development corporations. Since founding in 2007, Accela are providing high-quality, innovative products to over 3,000+ valuable customers in 38 countries. We run ISO9001-Quality-System daily, and certified by Tuv since 2010.* **418**

Ace Glass, Inc., 1430 N. West Blvd., PO Box 688, Vineland, NJ, United States 08360, 800-223-4524, fax: 800-543-6752, e-mail: sales@aceglass.com, Internet: www.aceglass.com *Ace Glass Incorporated has been a leader and innovator of scientific glassware, lab equipment and glass apparatus for over 80 years. Ace Glass provides a wide variety of quality U.S. manufactured standard and custom scientific glassware, including reactors engineered to any customer specifications from 100mL-200L.* **518**

ACS Career Fair Recruiters

ACS Career Consultants	**2028**
Aramco Services Company	**1825**
Brewer Science, Inc.	**1927**
Central Intelligence Agency (CIA)	**1931**
Getson & Schatz, P.C.	**2026**
Gilead	**1735**
Institute for Basic Science (IBS)	**1934**
KAUST	**1725**
Merck & Co.	**1925**
Nurix-Inc	**1929**
ORAU	**1935**
Sasol	**2034**

ACS Career Navigator, 1155 16th Street, NW, Washington, DC, United States 20036, 202-872-6031, e-mail: k_redmond@acs.org, Internet: https://www.acs.org/content/acs/en/careers/career-navigator.html **725**

ACS Committee on Chemical Health & Safety, P.O. Box 152329, San Diego, CA, United States 92195, 619-990-4908, Internet: www.acs.org/safety *The ACS Committee on Chemical Safety and the Division of Chemical Health and Safety provide this opportunity for you to learn more about chemical safety within the ACS and to have chemical safety experts answer your questions.* **1125**

ACS Division of Small Chemical Businesses (SCHB), 4344 Moorpark Ave., Ste # 1, San Jose, CA, United States 95129, 408-834-8597, fax: 408-351-7900, e-mail: expo-booth@acs-schb.org, Internet: www.acs-schb.org *The ACS Division of Small Chemical Businesses (SCHB) has objectives "To aid in the formation, development, and growth of small chemical businesses." SCHB helps chemists working in small enterprises, including self-employed, with the legal, social, educational, legislative, regulatory, and economic aspects of their unique professional status.* **1329**

ACS Education, 1155 16th Street, NW, Washington, DC, United States 20036, 202-872-6269, fax: 202-833-7732, e-mail: education@acs.org, Internet: www.acs.org/education *The ACS Education Division serves learners and educators by building communities and providing effective chemistry education resources, grants, communities, professional development opportunities, standards and guidelines. Stop by our booth to find information that can support your efforts to provide innovative, relevant, and effective chemistry education from kindergarten through professional education.* **725**

ACS Green Chemistry Institute, 1155 16th Street, NW, Washington, DC, United States 20036, 202-872-6102, fax: 202-776-8009, e-mail: gci@acs.org, Internet: www.acs.org/gci *The ACS Green Chemistry Institute® believes that innovation in sustainable and green chemistry and engineering (GC&E) is vital to solving environmental and human health challenges. Our mission is to catalyze and enable the implementation of GC&E throughout the global chemical enterprise and empower you to re-imagine a sustainable future.* **724**

ACS Meetings & Expositions, 1155 Sixteenth Street NW, Washington, DC, United States 20036, 800-227-5558, fax: 202-872-6128, e-mail: m_stevenson@acs.org, Internet: www.acs.org/meetings *The ACS Meetings booth displays information on current and future regional meetings and the spring and fall National Meetings. Register for a regional meeting or get information on submitting an abstract to a meeting in your region. The programming is diverse and exciting! Meet the volunteers who are planning these meetings at the booth. Visit the regional meetings website at www.acs.org/regionalmeetings for a tour of this year's conferences. Information on future national meetings will be on display.* **725**

ACS Member Insurance Program, 1155 16th Street, N.W., Washington, DC, United States 20036, 800-227-5558, ext. 6037, fax: 202-872-4435, e-mail: memins@acs.org, Internet: www.acs.org/insurance *The ACS Member Insurance Program is committed to offering quality comprehensive insurance plans to members and their families. Stop by the ACS station to learn more about the plans available such as Life and Health Insurance, Auto & Homeowners, Long Term Care, Professional Liability, Chemical Educators Legal Liability and more.* **725**

ACS Membership, 1155 16th St., NW, Suite OTH420, Washington, DC, United States 20036, 2028726062, Internet: www.acs.org/MemberHandbook *Visit Membership in the ACS Booth to pick up a copy of the 2017 Member Handbook and a booth raffle card. Visit at least 5 ACS Kiosks and return your completed card to be entered to win one of 10 prizes!* **725**

ACS Publications, 1155 16th Street, N.W., Washington, DC, United States 20036, 202-872-6862, fax: 202-872-6005, e-mail: s_jackson@acs.org, Internet: pubs.acs.org *ACS Publications is the leading publisher in chemistry and related sciences. Stop by our booth to receive free gifts and information on our newest journal, ACS Earth and Space Chemistry, and be sure to participate in our interactive author mosaic by using the hashtag #ACSmosaic. Visit ACS theater to meet Priestley Medalist Tobin Marks and learn about C&EN's Molecule of the Moment.* **725**

ACS Store, 1155 16th Street, NWWashington, DC 20036, United States, Phone: 800-ACS-5558 Fax: 202-872-6067, Internet: http://www.acs.org/store **725**

ACS Web Strategy & Operations, 1155 16th Street, NW, Washington, DC, United States 20036, 202-872-4548, e-mail: m_parker@acs.org, Internet: www.acs.org *ACS.org is getting a makeover! Our goal is to simplify the navigation and tell the ACS story in a more captivating way so you can find what you need faster and discover new things easier. Stop by the ACS Web kiosk to provide input and learn more.* **725**

AdValue Technology, 3158 S. Chrysler Ave., Tucson, AZ, United States 85713, 520-514-1100, fax: 520-747-4024, Internet: www.advaluetech.com *AdValue Technology specializes in areas of Alumina, Fused Quartz, Sapphire and Zirconia. Products range from Alumina and Silicon Dioxide Powders, Crucibles, Tubes & Rods, Plates & Discs, Sample Pans, UV Cuvettes, Quartz Wool, Ceramic Membranes, and Cerium Polishing Powders. We strive to be your valuable partner in Material Science!* **1224**

Advanced ChemBlocks Inc., 849 Mitten Rd., Suite 101, Burlingame, CA, United States 94010, (650) 692 2368, fax: (650) 560 6477, e-mail: sales@achemblock.com, Internet: www.achemblock.com *Advanced ChemBlocks Inc is a research-based manufacturer and world-wide supplier of various novel advanced building blocks and research chemicals for drug discovery. We focus on various advanced building blocks having biological and pharmacological bias. Please check our website www.achemblock.com for more information.* **1015**

Advanced Polymer Materials Inc., 2264 Chemin St. Francois, Dorval, QC, Canada H9P 1K2, 514-683-8488, fax: 514-683-2070, e-mail: gary.yu@apmpolymers.com, Internet: www.apmpolymers.com *We are a Canada based manufacturing company with R&D capability. We produce polymers and block copolymers for your R&D and production, such as controlled release formulation, tissue engineering, nanostructure formation, etc. We make functional block copolymers. We do contract research, custom synthesis and scaling-up according to your specification.* **1728**

Advion, 10 Brown Rd., Ithaca, NY, United States 14850, 607-379-4565, fax: 607-257-5761, Internet: www.advion.com *Advion is a leader in MS & synthesis solutions. The expression CMS is a high performance, compact, affordable single quad mass spectrometer. Its compact size allows it to fit in space-limited labs for direct access and immediate results for chemists requiring mass confirmation, reaction monitoring, QC and purity analysis. www.expressioncms.com* **1107**

AGI USA Inc., PO Box 21388, Lehigh Valley, PA, United States 18002-1388, (610) 691-2385, Internet: www.asahiglassplant.com *AGI is a world wide state- of-the-art scientific glassware manufacturer. Our proprietary Ring Baffle Reactor technology is the most efficient system in the world. Products include Rotary Evaporators, Thin Film and Short Path Evaporators, Pressure Reactors, Filter Reactors, Nutsche Filter Reactors, Molecular Distillation, Liquid-to-Liquid Extraction Columns and Mini Plants.* **1525**

AgileBio LLC - LabCollector, 5473 Keary Ville Road, Suite 255, San Diego, CA, United States 92123, 347-368-1315, Internet: www.labcollector.com *AgileBio develops LabCollector*

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V&P Scientific, Inc., 9823 Pacific Heights Blvd., Suite T, San Diego, CA, United States 92121, 858-455-0643, fax: 858-455-0703, e-mail: sales@vp-scientific.com, Internet: www.vp-scientific.com **213**

Vacuubrand, 11 Bokum Road, Essex, CT, United States 06426, 860-767-2562 ext. 125, fax: 860-767-2563, Internet: www.vacuubrand.com *VACUUBRAND offers exceptionally quiet, corrosion-resistant, oil-free vacuum pumps with ultra-long service intervals for labs, scale-up and OEM use. Products include both simple dry pumps and self-regulating, automated vacuum systems for critical evaporative applications. The line also includes the unique HYBRID pumps, which reduce oil-changes by 90%, even in corrosive applications. VACUUBRAND will also show corrosion-resistant digital vacuum gauges and controllers. New products include high flow-rate, chemical-resistant dry vacuum pumps for kilo-lab and pilot-scale applications.* **1519**

Vacuum Atmospheres Co., 4652 West Rosecrans Avenue, Hawthorne, CA, United States 90251, 310-644-0255, fax: 310-970-0980, e-mail: info@vac-atm.com, Internet: www.vac-atm.com *VAC has set the standards for gloveboxes and inert gas purification for over 50 years. Once again, our ongoing research and development has produced a proven revolutionary design. NO REGENERATION required by the user. Please visit us in booth 1207.* **1207**

Vacuum Process Engineering, Inc., 110 Commerce Circle, Sacramento, CA 95815, United States, 916-925-6110, Internet: http://www.vpei.com 1906

Vacuum Technology Inc., 15 Great Republic Drive, Unit #4, Gloucester, MA, United States 01930, 978-879 4302, fax: 978-879 4387, e-mail: sam.cai@vti-glovebox.com, Internet: www.vti-glovebox.com *Based in Gloucester, Massachusetts, Vacuum Technology Inc. builds and services the glove box needs of educational and industrial clients worldwide by integrating best–in-class components sourced from Europe, Asia, UK and the USA. Along with standard offerings, we proudly highlight our engineering talent and customer-centric customization shop.* **1814**

Vapourtec Ltd., Unit 16, Park Farm Business Centre, Fornham St Genevieve, Suffolk IP28 6TS, United Kingdom, 44 1284 728659, fax: 44 1284 728352, e-mail: duncan.guthrie@vapourtec.com, Internet: http://www.vapourtec.com *Vapourtec manufacture two series of flow chemistry systems:*
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Wavefunction, Inc., 18401 Von Karman, Suite 370, Irvine, CA, United States 92612, 949-955-2120, fax: 949-955-2118, e-mail: sales@wavefun.com, Internet: www.wavefun.com *Wavefunction, Inc.: Molecular Modeling Software provider for chemistry research and education.* **709**

Welch by Gardner Denver, 1601 Feehanville Drive, Suite 550, Mount Prospect, IL, United States 60056, 847-676-8800, fax: 847-677-8606, Internet: www.welchvacuum.com **1200**

Westcoast Separation, LLC, 3201 Corte Malpaso, #310, Camarillo, CA, United States 93012, 805-504-7767, Internet: www.westcoastseparations.com *Westcoast Separations specializes in chromatographic technologies for method development, analysis and purification of small molecules. We offer screening of columns, method development and purification for chiral and achiral molecules. We combine the benefits of analytical and preparative HPLC and Supercritical Fluid Chromatography (SFC) to achieve separation goals and results.* **1632**

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Workrite Uniform Company, 1701 North Lombard St., Oxnard, CA, United States 93030, 800-521-1888, fax: 805-483-0678, e-mail: info@workrite.com, Internet: www.workritefrcp.com **1813**

WuXi AppTec (Shanghai) Co. Ltd., 288 Fute Zhong Road, Waigaoqiao Free Trade Zone, Shanghai, China 200131, e-mail: hr@wuxiapptec.com, Internet: www.LabNetwork.com *LabNetwork, a WuXi AppTec company, is a global eCommerce platform connecting suppliers and buyers of research products. Backed by WuXi AppTec's expertise in R&D, sourcing, quality control, warehousing and logistics, LabNetwork brings high-quality compounds from WuXi's network of qualified providers to the global chemistry/R&D community.* **1601**

Wyatt Technology Corp., 6300 Hollister Avenue, Santa Barbara, CA, United States 93117, 805-681-9009, fax: 805-681-0123, e-mail: info@wyatt.com, Internet: http://www.wyatt.com *Wyatt Technology is the recognized leader in instrumentation for determining the absolute molar mass, size, charge and interactions of macromolecules and nanoparticles in solution. These tools include: in-line multi-angle static*

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Joseph M. DeSimone has published over 300 scientific articles and has over 150 issued patents in his name with over 80 patents pending. In June 2016, DeSimone was recognized by President Barack Obama with the National Medal of Technology and Innovation. DeSimone is one of less than twenty individuals who have been elected to all three branches of the U.S. National Academies: National Academy of Medicine (2014), National Academy of Sciences (2012) and the National Academy of Engineering (2005).

DeSimone is the co-founder of several companies including Micell Technologies, Bioabsorbable Vascular Solutions, Liquidia Technologies and Carbon. DeSimone received his B.S. in Chemistry from Ursinus College in Collegeville, PA and his Ph.D. in Chemistry from Virginia Tech. He currently resides in Monte Sereno, California.

AND

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Andrews has been the recipient of an NIH Fellows Award for Research Excellence, an Eli Lily Outstanding Young Analytical Chemist Award, an American Parkinson's Disease Association Research Award, and a Brain and Behavior Research Foundation Independent Investigator Award. She is a member of the American College of Neuropsychopharmacology, International Society for Serotonin Research vice president, an advisory board member for the International Society for Monitoring Molecules in Neuroscience, and serves as Associate Editor for *ACS Chemical Neuroscience*.

Andrews earned her B.S. in chemistry from the Pennsylvania State University and received her Ph.D. in chemistry as a U.S. Department of Education Fellow working at the National Institute of Mental Health. There, she was also a postdoctoral fellow and senior staff fellow.

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Newscripts

The ketchup problem

We've all waged battle with a glass ketchup bottle at some point—fighting to get that stubborn tomato slurry to pour without splattering.

The process can be frustrating because ketchup is a yield-stress fluid, says Anthony Stickland, a chemical engineer at the University of Melbourne.

Like other yield-stress fluids, ketchup is a suspension of solid particles in liquid. "The solids are concentrated enough that the particles form an interconnected network that can withstand a load or a force," Stickland tells Newscripts. So under small amounts of stress, the fluids behave like solids. But once that force exceeds a threshold—the yield stress—the materials start to flow like a liquid.

That's why ketchup bottles sometimes need a firm whack to get the sauce moving.

Stickland recently outlined a three-step process to coax out the condiment. First, shake the bottle with the lid on to evenly mix the ketchup. This gets rid of any dried-out sauce or settled solids that increase the yield stress. Next, with the lid still on, invert the bottle to get the ketchup into the neck. Finally, remove the lid and slowly tilt the bottle so the weight of the condiment pushes it out.

Tilting too fast can lead to splattering because the viscosity of some yield-stress fluids decreases when forces are applied quickly, a phenomenon called sheer thinning. "If you push really hard, it becomes almost like water," Stickland says.

So why does Stickland know so much about getting ketchup out of a bottle? His research focuses on industrial versions of the problem, such as pumping wastewater sludge or mineral tailings.

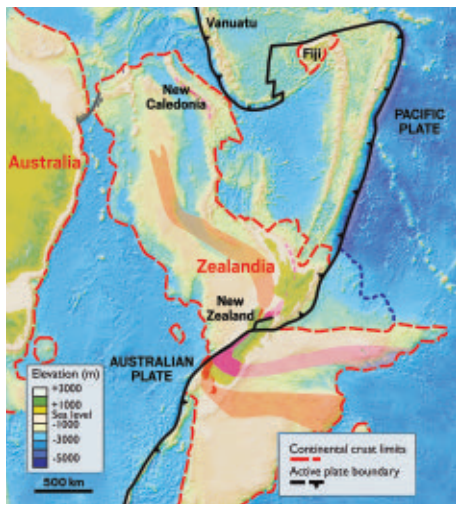
Meet Zealandia

At your next cookout, once you've effortlessly extracted your ketchup, you can further impress your guests with some geological trivia: There is an eighth continent to the east of Australia, some geologists say.

It's called Zealandia, and its 4.9 million-km² area contains New Zealand and some French and Australian islands. But you won't be able to see it just looking at a map or globe.

"The key reason why Zealandia has not been recognized traditionally is 94% of it is underwater," says Vaughan M. Stagpoole of GNS Science.

Despite mostly being submerged, Zealandia has all the characteristics of the continents we know and love. Stagpoole and several colleagues lay out the case for Zealandia's continental membership in a recent paper (*GSA Today* 2017, DOI: 10.1130/gsatg321a.1).



Number 8: Most of Zealandia is a submerged continental shelf.

Basically, the land masses and submerged continental shelf of Zealandia are geologically distinct from the oceanic crust surrounding them. In general, continental crust is thicker and is less dense than oceanic crust.

One interesting feature of Zealandia is that a tectonic plate boundary runs through it. The northwestern portion of the continent is on the Australian plate, and the southeastern bit is on the Pacific plate. "The tectonic activity at the plate boundary is pushing New Zealand up," Stagpoole tells Newscripts. "If it weren't for the frequent earthquakes here, most of New Zealand would be underwater."

Michael Torrice wrote this week's column. Please send comments and suggestions to newscripts@acs.org.

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