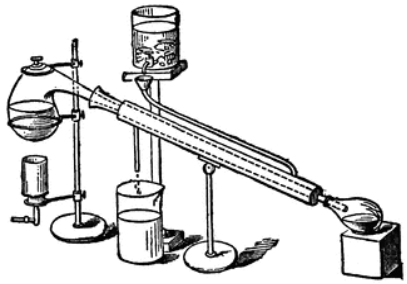
SOUTHWEST RETORT



SEVENTIETH YEAR **FEBRUARY 2018**

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and Chemistry in this area

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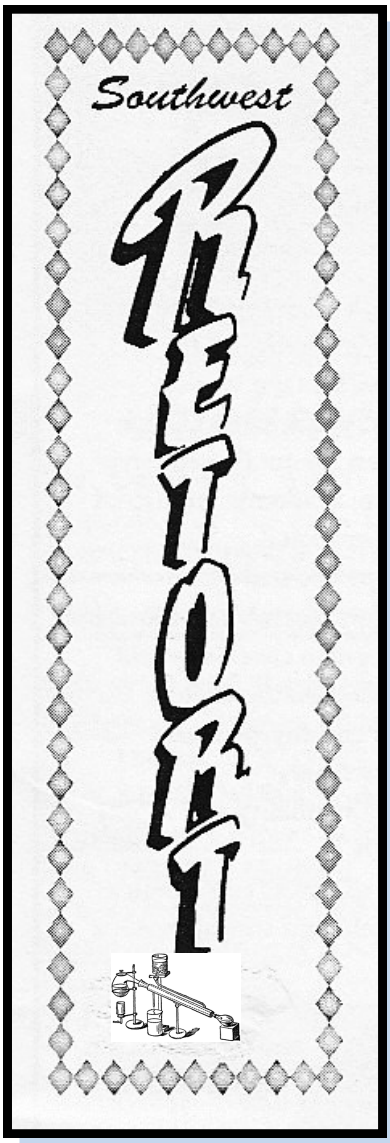

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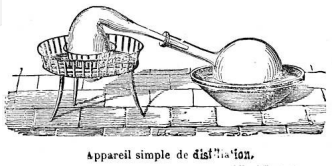

EMPLOYMENT CLEARING HOUSE

Job applicants should send name, email, and phone, along with type of position and geographical area desired; employers may contact job applicants directly. If you have an opening, send your listing, including contact info for your company, to retort@acsdfw.org. Deadlines are the 7th of each month.

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Requirements:
Bachelor's degree or higher (Chemistry/Biology/Biochemistry or similar background preferred); Excellent interpersonal and communication skills; Excellent reading, speaking, and writing skills in business English; Good arithmetic skills and attention to details required; Proficiency in the use of Microsoft Word, Excel, PowerPoint, and Outlook required; English/Chinese bilingual preferred; Ability to work independently required. Prior sales, marketing, or accounting experience are considered a plus.

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FIFTY YEARS AGO IN THE SOUTHWEST RETORT

The two ACS tour speakers for February are Dr. Norman Hackerman, President of the University of Texas at Austin, and Dr. John K. Stille of the University of Iowa. Dr. Hackerman's lecture topics will be either "Fuel Cells" or "Molecular Structure and Corrosion." Dr. Stille's topics include four on polymer chemistry, one on organometallic chemistry, and one on heterocyclic chemistry.

Hugh D. McAfee has been named by Dean of Science Peter Girardot to be acting head of the UT-Arlington chemistry department. Mr. McAfee is an associate professor of chemistry, who has been on the faculty 21 years. At the Mobil Research and Development Laboratories in Dallas, Mr. Ellis Bray has been appointed acting supervisor of the Petroleum Geochemistry Section. Bray has specialized in the application of infrared and mass spectrometry to geochemical problems. He has made significant contributions to research on the origin of oil and the identification of source rocks. Also at Mobil Dr. Peggy M. Dunlap has been promoted to research associate. She is currently studying the interfacial tension between water and hydrocarbons.

At TCU Dr. Clifford Venier has recently received a PRF Type G grant to study "Reactions of Nucleophiles with Sulfines." Dr. Henry C. Kelly recently presented a research seminar at the University of Arkansas, while Dr. Manfred G. Reinecke presented a research seminar at the University of New Hampshire. Dr. John C. Bailar, Jr. of the University of Illinois will give a Welch Lecture at Austin College on Feb. 12.

At Trinity University in San Antonio Dr. Ben Plummer received a research grant to study acenaphthylene photo dimers. At Sam Houston State College Dr. Benjamin Widom from Cornell gave the Welch Lecture. At the University of Houston Drs. Ralph Becker, Raymond B. Seymour, and W. W. Wendlandt are currently writing books which will be published this year. At Texas Tech Dr. Yuzura Murata is a new post-doc with Dr. Henry Shine. Dr. John Marx gave a paper at the Second International Natural Products Symposium held in Kingston, Jamaica.

At Baylor the Welch Lecture was given by Dr. Robert S. Hansen of Iowa State University. Faculty member Dr. Thomas C. Franklin gave a talk to the South Texas Section of the Electrochemical Society at the Geo Club in Houston. He also gave seminars at TCU and at East Texas Baptist College.

contributed by
E. Thomas Strom

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And Another Thing...

Bring It On Home

By Denise L. Merkle, PhD

Who hasn't been at home at some point and thought, 'I need an X! Where is that X?' only to realize that X is safely tucked away in the lab. Well, drat. No X for you. Since it is intriguing to know what people want to do with their spare time, scientists were asked 'What X do you have in the lab that you wish you had at home?' Answers were definitely interesting.

I would really like to have a dry Nitrogen source. Inert atmospheres are so handy for storing fermented beverages and for preventing rust on garden tools. A tank, some tubing, a regulator and a nozzle- I'd be set. Why is dry N_2 not a standard feature? In many environments, lack of O_2 is excellent for impeding microbial growth, so a nitrogen flush is very helpful. One survey respondent, however, took aseptics to a new level, suggesting an autoclave would be useful to "really kill some stuff"[1]

Once you've flushed your materials with dry N_2 (g), you'll hope Parafilm is available. Which it can be - easily! Buy it on amazon.com. 250ft of Parafilm is a lot of stretchy, sealed up happiness, a must-have in the home.

How about stir plates? It's a lot easier to perfect your chocolateering with a gizmo that allows precise control of both applied heat and the speed of those handy dandy stir bars - from the lab to the dessert tray.

It's not amazing that quite a number of chemists cook like crazy and that they want liquid N_2. As we all know, N_2(l) has all sorts of applications - and when it's not making ice cream or other culinary delights, it has marvelous entertainment value. But don't forget water baths! H_2O baths are a must "for the odd sous vide endeavor"[2].

Do you want to reduce your sauce? A Rotovap would be very useful for removing that unwanted liquid. Make sure you have a vacuum pump to accelerate your rotovapping, and just think how a vacuum pump could open up new vistas of utility in the home. Sometimes a vacuum cleaner just doesn't have enough resolution.

Perhaps you have more of an engineering mindset? You might want, as did one survey participant, a mill and a lathe. There are few things so gratifying as heading to the garage to whip up a part that you're interested in trying. 3-D printers, anyone? Also exciting for the scientist's materials dreams.

Serious materials dreamers need X-ray diffractometers and spectrophotometers. How will you know what you have to work with, if you can't analyze it properly? Pop that unknown substance into the sample chambers, and soon it is unknown no longer. Analyze everything in the home - rocks from the yard, the fabric of new clothing, spooge on the fish tank, etc. If characteristics determine function, new applications await with every structural determination.

Or, if your home is seriously mired in hard-core precision, perhaps you want to go a bit beyond milling and lathing, and construct your own atomic clock. For this, you'd have a NIST WWV-linked frequency standard[3]. Accurately measure any frequency in the home - and tune your atomic clock to the world standard.[4] (I'd likely have to retard any clock by 10minutes, to match my intrinsic delay, but NIST may not offer standards for that.)

So, there you have it, an unscientific study of scientists' hopes for the home. Many, thanks to everyone who sent Wish Lists, and apologies to anyone whose response was missed. Although all the wishes may not be fulfilled, I wonder most if a local scientist finally amassed enough parts to build a synchrotron in the backyard. Perhaps, though, the construction delay was more rooted in overcoming spousal resistance than in gathering enough bits and pieces.

You may not get your synchrotron, but VISA and an online vendor can provide almost everything else. It's good to be a scientist in 2018.

1) Dr. M.

2) Dr. T

3) https://www.nist.gov/pml/time-and-frequency-division/time-services/wwv-and-wwvh-digital-time-code-and-broadcast-format

4) Atomic Physicists - sheesh

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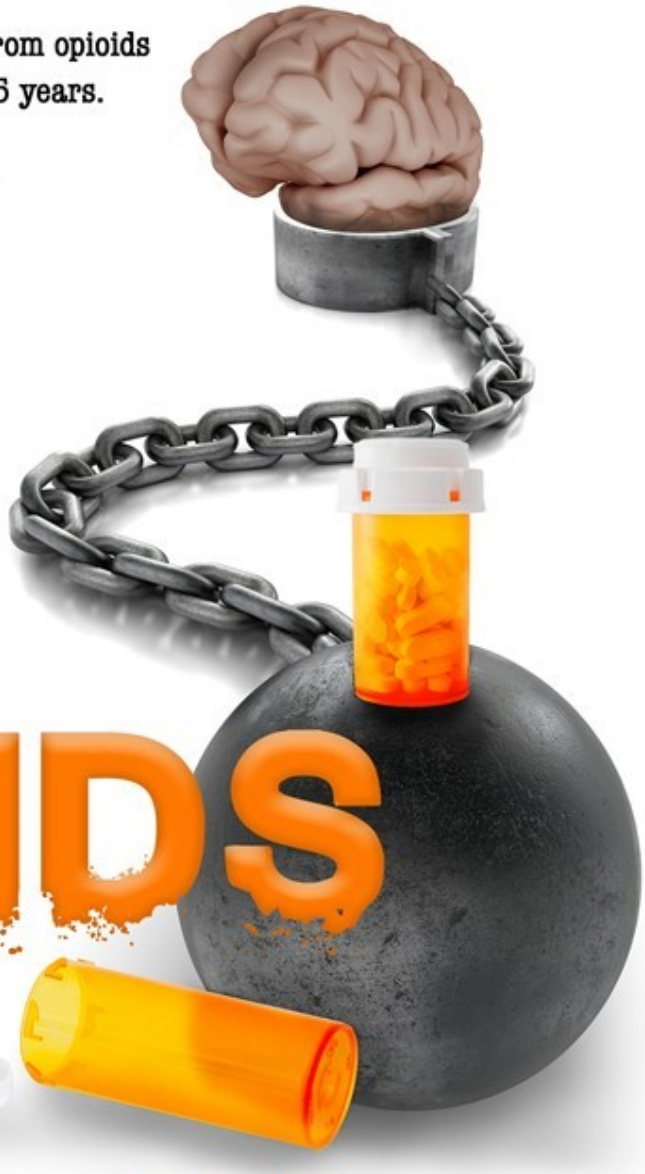

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ACS PROGRAM-IN-A-BOX

WHERE
8150 N. Central Expy, 10th Fl., Dallas

TIME
5:45pm (Come early for food!)

WHEN
Tuesday, February 27th, 2018

CONTACT
Kirby Drake, kirby@klemchuk.com

In Memoriam of Dieter Cremer (1944 - 2017)

SMU 27th Austin Symposium on Molecular Structure and Dynamics at Dallas, March 3-5, 2018 ASMD@D

Welcome To ASMD@D - The Somewhat Different Conference
http://www.austinsymposium.org/

The **27th Austin Symposium on Molecular Structure and Dynamics at Dallas (ASMD@D)** will be held at *Highland Dallas Curio Hotel* close to the SMU campus from **March 3-5, 2018.**

The ASMD@D 2018 is dedicated in memoriam of Dieter Cremer (1944 - 2017), who served as Chairman of the 2012, 2014, and 2016 ASMD@D meetings vitalizing the symposia with many new refreshing ideas and inspiring scientific discussions. The meeting will be organized in the spirit of previous symposia: Meet international experts - Listen and discuss - No parallel sessions - A place where important interdisciplinary work can start - A place where experimentalists and computational chemists can join forces - A place where graduate students and postdocs can create networks for their future academic career.

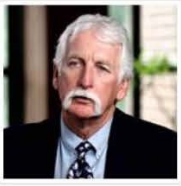
The conference theme will be ***"Experiment, Theory and Beyond."***

Featured speakers are

Professor Steven Boxer
Structure and Function of Biological Systems

Professor Ken Houk
Computer Modeling of Organic/Biochemical Systems

Professor William Jorgensen
Computer-aided Design & Development of Therapeutic Agents



Professor K. V. Lakshmi
Pulsed EPR/Solids NMR Spectroscopy

Professor Kenneth Leopold
High Resolution Microwave Spectroscopy

Professor Leo Radom
Computational Quantum Chemistry

Professor Markus Reiher
Quantum Chemistry & Quantum Computing

Dr. Matthias Rupp
Machine Learning for Atomistic Systems

(For the list of all confirmed speakers, please see:
SPEAKERS)

We hope to see you in March,

Professor Elfi Kraka
Chair of the Organizing Committee of ASMD@D
Computational and Theoretical Chemistry Group (CATCO)
http://smu.edu/catco/, SMU, Dallas, Texas, USA

FORT WORTH OPERA

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— *NPR*

Don Pasquale

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From the ACS Press Room

Mind-controlling molecules from wasp venom could someday help Parkinson's patients

Ampulexins: A New Family of Peptides in Venom of the Emerald Jewel Wasp, Ampulex compressa
Biochemistry

After being stung by a parasitic wasp, the American cockroach loses control of its behavior, becoming host to the wasp's egg. Days later, the hatchling consumes the cockroach alive. While this is a gruesome process for the cockroach, scientists now report in ***Biochemistry*** the discovery of a new family of peptides in the wasp's venom that could be key to controlling roach minds, and might even help researchers develop better Parkinson's disease treatments.

Scientists have long studied venoms, such as that of the wasp, seeking out novel and potent molecules to treat disease, among other applications. In the case of the enigmatic wasp Ampulex compressa, it uses its venom in a two-pronged approach against the cockroach, with an initial sting to the thorax to paralyze the front legs and a subsequent sting directly to the brain. This second sting causes the roach first to vigorously groom itself, then to fall into a state of lethargy, allowing the wasp to do whatever it wants. This immobile state resembles symptoms of Parkinson's disease, and both may be related to dysfunction in the dopamine pathway. In this study, Michael E. Adams and colleagues wanted to identify the ingredients in wasp venom that dictate this behavior.

The researchers milked wasps for their venom and then analyzed the components using liquid chromatography and mass spectrometry. They identified a new family of alpha-helical peptides and named them ampulexins. To test their function, the team injected the most abundant venom peptide into cockroaches. Afterward, the bugs needed, on average, a 13-volt electric shock to the foot to get them moving, while an average of 9 volts sufficed prior to the injection, suggesting the peptides help the wasp immobilize its prey. Future work will focus on identifying cellular targets of ampulexins, and potentially generating a useful animal model for the study of Parkinson's disease treatments.

The authors acknowledge funding from the United States-Israel Binational Science Foundation, the University of California, Riverside Office of Research and Economic Development and the University of California Agricultural Experiment Station.

DFW Section Events

Save the date!

51st ACS DFW Meeting in Miniature

Saturday, April 28, 2018

Southern Methodist University

Undergraduate and graduate oral sessions

Volunteer judges will be needed

Watch your email and the Retort for more details.

Contact Organizers Dr. Isaac Garcia-Bosch (igarciabosch@mail.smu.edu) or Dr. Alex Lippert (alippert@smu.du) for more information.

Whiskey Distillery Tour and Tasting

Wednesday, March 28, 2018, 6 pm

Firestone & Robertson Distilling Co.

901 W Vickery Blvd, Fort Worth TX 76104

www.FRdistilling.com

Join the DFW Local Section for a tour of the first craft bourbon and whiskey distillery in North Texas. A tasting will be available for attendees that are 21 and over. The head distiller will then join us for an optional Dutch treat dinner at a nearby restaurant following the tour.

Around the Area

Texas Tech University

Prof. **Jonathan Sweedler** (University of Illinois at Urbana-Champaign) is the guest speaker at Texas Tech University for the Fourth Dasgupta Lecture Series, Feb 7th & 8th. His research focus is on developing new approaches for assaying small volume samples, and in applying these methods to study novel interactions between cells. He is presenting a general audience lecture entitled "Understanding the brain a cell at a time: from new measurement tools to chemical insights" on Feb 7 at 5 PM and a technical lecture "D-amino acids in our brain: what are they doing and how did they get there?" on Feb 8th. This lecture series was endowed by students, colleagues and friends of former TTU Professor Purnendu K. "Sandy" Dasgupta. Prof. Dasgupta plans to be in attendance.

UTA

Martin Pomerantz, Professor Emeritus, in the Chemistry and Biochemistry Department at the University of Texas at Arlington has received the prestigious Albert Nelson Marquis Lifetime Achievement Award from Marquis Who's Who for his longstanding dedication, leadership, and excellence in his profession as an organic and polymer chemist.

TWU

The Department of Chemistry and Biochemistry at Texas Woman's University (TWU) has recently been recognized by the Association of American Colleges and Universities (AAC&U) for its incorporation of civic engagement and social responsibility into the chemistry and biochemistry undergraduate curriculum. TWU was one of nine institutions featured in Civic Learning in the Major by Design (peerReview 19-4, Fall 2017, 28-30) and the only hard science department of 23 institutions recognized as model departments for educating students to apply a civic lens to their discipline. For more information, please visit https://www.twu.edu/news-events/news/texas-womans-university-chemistry-program-earns--top-national-recognition-/.

University of Arkansas

On the Go

Feng Wang gave an invited talk, "Modeling hydration of simple ions on the MP2 potential energy surface with molecular mechanics force fields", Symposium on Contemporary Computational Chemistry." 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, Nov. 2017.

Several members of the Fritsch group participated in the Gordon Research Seminar on Electrochemistry (January 6-7, 2018) and the Gordon Research Conference on Electrochemistry (January 7-12, 2018) in Ventura, CA. The poster presentations are:

Aaron Nicholson, Foysal Khan, and Ingrid Fritsch, Fundamental studies of circular redox- magnetohydrodynamic microfluidics: Toward small-scale, loop based chemical separations and sampling.

Benjamin J. Jones and Ingrid Fritsch, Conducting copolymers from aqueous Co-electropolymerization of two thiophene-containing monomers with different functional groups and subsequent film conjugation.

Foysal Z. Khan, David N. Parette, and Ingrid Fritsch, Optimizing polymer-immobilized, redox- magnetohydrodynamics (R-MHD) pumping for microfluidics systems.

Mahsa Lotfi Marchoubeh, Mengjia Hu, and Ingrid Fritsch, Challenges of simultaneous measurement of catecholamines in mixtures: Steps toward neural probes suitable for in vivo analysis.

Jazlynn Sikes, Isabelle Niyonshuti, Jingyi Chen, and Ingrid Fritsch, Investigations of variations in electrochemical signals from impacts by silver nanoparticles of differing shapes.

Publications

Sumana Venkat, Jourdan Sturges, Alleigh Stahman, Caroline Gregory, Qinglei Gan, Chenguang Fan. Genetically incorporating two distinct post-translational modifications into one protein simultaneously. ACS Synth. Biol. 2018. doi: 10.1021/acssynbio.7b00408. [Epub ahead of print].

T. Ryan Rogers, Feng Wang. Performing the Millikan experiment at the molecular scale: Determination of atomic Millikan-Thomson charges by computationally measuring atomic forces. J. Chem. Phys., 2017, 147, 161726.

Jicun Li, Feng Wang. Accurate prediction of the hydration free energies of 20 salts through adaptive force matching and the proper comparison with experimental references. J. Phys. Chem. B, 2017, 121, 6637.

Honors and Awards

Mahsa Lotfi Marchoubeh placed second in the Fulbright College 3 minute thesis competition January 22-26. The top finisher from each col-ege will advance to a university-wide final on February 2. The competition celebrates discoveries made by graduate students and encourages them to communicate the significance of their research to the broader community in language that is understood by the general public. The competition is sponsored by the Graduate School and International Education and was founded by the University of Queensland in 2008. The event will serve as the capstone to Graduate Education Week, which kicks off January 29. More can be found in the UA Newswire article located at http://bit.ly/2j32mP9

Emeritus Professor **Peter Pulay** was awarded the J. Clarence Karcher medal January 19, 2018. He was the Karcher-Barton Lecturer at the University of Oklahoma, Norman. The medal honors J. Clarence Karcher (1894-1978), who was a distinguished scientist, innovator and alumnus. His pioneering development of the reflection seismograph resulted in the discovery of energy resources for much of the world.

Nominations are invited for 2018 Wilfred T. Doherty and Werner Schulz awards

Nomination forms and additional information are available online at http://dfw.sites.acs.org/localsectionawards.htm. Nominations are due by May 15, 2018. Each nomination should contain completed nomination form, cover letter highlighting the nominee's accomplishments, and a copy of the CV. One seconding letter may accompany nominations. The nomination package should be sent by email as a single pdf file to Stephen Starnes (Stephen.Starnes@tamuc.edu). Nominations remain active for five years but should be updated annually.

The Doherty Award is given for excellence in chemical research or chemistry teaching, meritorious service to ACS, establishment of a new chemical industry, solution of pollution problems, and advances in curative or preventive chemotherapy. Nominees may come from industry, academia, government, or small business. The nominee should be a resident member in the area served by the DFW Section, and the work should have been done here. The award is $1500 and an engraved plaque. A photo of the Doherty Award winner will be displayed permanently in the Gallery of Doherty Award winners, Berkner Hall, UT-Dallas.

The Schulz Award is given to high school chemistry teachers, who, like the late Dr. Werner Schulz, bring that something extra to the teaching of chemistry. The nominee and/or nominator need not be ACS members. Nominees should show excellence in chemistry teaching as demonstrated by testimonials from students and fellow teachers, results in student competitions, and diligence in updating and expanding scientific/teaching credentials. A photo of the Schulz Award winner will be displayed for one year at the Perot Museum of Nature and Science in Dallas, and then displayed permanently in the Gallery of Schulz Award winners, Science Bldg., Tarleton State University. A traveling plaque stays at the winner's high school for the year of the award. Winners will normally receive their awards and give their lectures at a fall meeting of the section.

Remember, a continuous flow of nominations is needed to maintain the quality of awards.

From the ACS Press Room

The potential impact of hydraulic fracturing on streams

Water Stress from High-Volume Hydraulic Fracturing Potentially Threatens Aquatic Biodiversity and Ecosystem Services in Arkansas, United States

Environmental Science & Technology

Concerns over hydraulic fracturing, an oil and gas extraction method that injects millions of gallons of freshwater and chemicals into shale, have largely focused on potential impacts on water quality. But, as scientists report in ACS' journal **Environmental Science & Technology**, "fracking" operations could have impacts on water quantity because they are withdrawing these large amounts of water from nearby streams, which house aquatic ecosystems and are used by people for drinking and recreation.

On average, more than 5 million gallons of freshwater is used to fracture one gas well in the U.S. That's more than enough to fill seven Olympic-size swimming pools. Small streams are a major source of water for these operations. Some of these streams also provide drinking water for communities and homes for species with already declining populations. However, little is known about the amount of water that can be sustainably withdrawn from these sources. Sally Entrekin and colleagues wanted to flesh out this picture for the Fayetteville Shale play, an active gas field in Arkansas where more than 5,000 gas wells were drilled using fracking techniques between 2004 and 2014.

The researchers estimated the water stress that hydraulic fracturing might place on streams in the gas field based on water usage and timing for fracturing wells and data on nearby stream flow rates. The streams in the area studied help supply drinking water to thousands of people in the region and are home to 10 aquatic species that are declining at a concerning rate. The team's calculations revealed that freshwater usage for fracking could potentially affect aquatic organisms in 7 to 51 percent of the catchments, depending on the month. If 100 percent of the wastewater were recycled, the potential impact drops, but 3 to 45 percent of catchments could still be affected. The researchers conclude that improved monitoring and access to water withdrawal and streamflow data are needed to ensure protection of streams as drinking water sources and valuable habitat in the future.

The authors acknowledge funding from the Science for Nature and People Partnership (SNAPP), a collaboration of The Nature Conservancy, the Wildlife Conservation Society and the National Center For Ecological Analysis and Synthesis (NCEAS) at the University of California Santa Barbara.

From the ACS Press Room

Lab-grown horns and tusks could stop poaching

Can synthetic horns and tusks offer hope against poachers?
Chemical & Engineering News

Scientists are making mimics of rhino horns and elephant tusks, hoping to drive down the prices of these items on the black market and discourage poaching. But many conservation groups argue that it could have the opposite effect, according to an article in Chemical & Engineering News (C&EN), the weekly newsmagazine of the American Chemical Society.

Melissa Pandika, special to C&EN, reports that in 2015, more than a thousand rhinos were poached in Africa, and every year, about 27,000 African elephants suffer the same fate. Rhino horns are prized for their purported medicinal benefits, and both rhino horns and elephant tusks are often turned into jewelry and other decorative objects by artisans. All of this is happening despite a United Nations treaty prohibiting the global commercial trade of rhino horn and ivory.

Now, companies are betting that flooding the market with synthetic, lab-grown mimics will decrease poaching, making it less worthwhile for hunters. Two companies are growing rhino horns from stem cells, and other researchers are investigating ways to build elephant tusks. Many conservationists, however, say that hunters could try to pass off their wares as being biofabricated. But the scientists propose introducing DNA barcodes or microscopic features to distinguish synthetics from the real thing. Animal conservation groups also argue that the new materials could simply expand demand for such items, creating an inexpensive market existing in parallel with poached items. Alternatively, poached products could become even more desirable, showing that the customer can afford the risk of getting caught. Although the controversy continues, there's one thing both sides can agree on — the killing of these majestic, endangered animals must end.

From the ACS Press Room

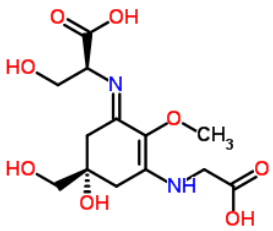
Getting ready for the summer sun with 'green' sunscreens

Photosynthetic Production of Sunscreen Shinorine Using an Engineered Cyanobacterium

ACS Synthetic Biology

Although it's been a tough winter for many people in the U.S., summer is coming. And that means backyard barbeques, fun on the beach and, of course, slathering on sunscreen. But one particular environmentally friendly sunscreen ingredient has been difficult to obtain — that ingredient, shinorine, could only be harvested from nature. Scientists now report in ACS **Synthetic Biology** the laboratory production of that compound.

Sunscreen is key to protecting the skin from carcinogenic UV radiation. However, some synthetic sunscreen components can accumulate in aquatic environments and potentially cause harm by acting as hormone disruptors. One alternative to these ingredients is the biodegradable sunscreen compound shinorine, a UV-absorbing substance produced naturally by cyanobacteria and marine algae. The shinorine currently found in commercially available sunscreens comes from red algae gathered from the sea, but the yield can vary seasonally and geographically, limiting supply. So, Yousong Ding and colleagues sought to develop a more reliable source of shinorine by bringing production out of the wild and into the laboratory.



The team selected a strain of freshwater cyanobacteria, *Synechocystis*, as a host cell for shinorine expression because it grows quickly, and it is easy for scientists to change its genes. Next, they mined the cluster of genes responsible for the synthesis of shinorine from a native producer, the filamentous cyanobacterium Fischerella. The researchers then inserted these genes into *Synethcocystis*. At first, the production was dismal, three times lower than Fischerella production. But adding extra promoters to the gene cluster increased production ten-fold. Finally, the team exposed control cells and those expressing shinorine to UV radiation. No growth differences were observed with UV-A light. But control cells experienced an obvious decline in population from UV-B exposure. The researchers say that in the other cells, shinorine acted as sunscreen against UV-B light, which helped the cells live and grow better.

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From the editor

Best regards,
Connie