

# SILICON VALLEY CHEMIST



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## Picnic Message

Our Silicon Valley ACS festive summer picnic has all the trappings of a picnic with a barbecue feast, wine, and beer in a lovely outdoor setting. But it is a lot more. It is also an opportunity to celebrate – our long-time ACS members, our section's service award-winners, and each other, particularly as we relish personal interactions once again. This SVACS event is family-friendly with children eating and playing outdoors while their families socialize.

One phase of the Saturday event is a wine- and beer-tasting, planned and served by our section's 'sommelier', Peter Rusch, and master-

*continued on next page*

## 2024 Silicon Valley ACS Picnic and Awards

A family-friendly event, please join us for our annual picnic and awards ceremony! [Download flyer](#) (PDF)

**Date and Time:** July 13, 2024, 4-7pm

- 4:00-5:00 pm: Wine & Beer Tasting with hors d'oeuvres
- 5:00 pm: Awards & Recognitions – *Silicon Valley ACS Ottenberg Award* and celebrating 50-, 60- and 70-year ACS members
- BBQ dinner will immediately follow Awards & Recognitions, catered by Armadillo Willy's

**Location:** Cuesta Park Group BBQ Areas #1-2, Mountain View ([view map, get directions](#))

**Advanced registration required by the end of the day, July 10, 2024**

**Cost:** \$10.00. Children: free. Payment by cash or check at the door. If paying by check, please make it out to "Silicon Valley ACS."



Silicon Valley ACS  
Annual Picnic & Awards

Come celebrate together with  
wine- & beer-tasting, good food & awards

Saturday, 13 July 2024  
4-7 pm  
Cuesta Park Group BBQ  
Areas #1 & #2, Mountain View

ACS  
Silicon Valley

For information go to  
<https://www.siliconvalleyacs.org/event/2024-annual-bbq-picnic-and-awards-ceremony/>  
Registration deadline extended to end of the day on July 10.  
Registration is required to make sure there is plenty of food.

*Picnic Message, continued from front page*

brewer, Matt Greaney. Come learn about new beverages in good company.

The highlight of our Saturday together is recognizing both extraordinary contributors to our section and our long-time ACS members. The Silicon Valley ACS honors outstanding volunteerism in several areas with a number of awards. Come meet the heroes and see the village that makes our section so effective for chemists and the community.

We then honor our section's members with fifty or more years of membership in the American Chemical Society. The esteemed attendees recount their histories and retrospective lessons - interesting and inspiring storytelling about the

trials, tribulations, and accomplishments in their chemistry careers.

The picnic provides us the opportunity to meet new people and see old friends, to talk about research and lives in the Bay Area, and to relish being in the company of like-minded folks while broadening our view with others' experiences.

This year's picnic is on Saturday, July 13th in Mountain View's Cuesta Park. Registration information is in this July newsletter. Don't wait long to register as orders get placed with our caterer on July 10th.

Share the colorful SVACS picnic poster on this newsletter front page with friends and family. We look forward to seeing you all there!

## Frances H. Arnold awarded the 2025 ACS Priestley Medal

"The American Chemical Society (ACS) is proud to announce that **Frances H. Arnold** is being awarded the 2025 **Priestley Medal**. This award is the highest honor bestowed by ACS, and it annually recognizes an individual for distinguished service to chemistry. Arnold is being honored "for her pioneering contributions to the development of directed evolution as a method for chemical and biological design." She was also awarded the Nobel Prize in chemistry in 2018 for the technique."

[Read ACS News Release](#) | [Caltech News](#)



*Caltech Linus Pauling Professor of Chemical Engineering, Bioengineering and Biochemistry; Director, Donna and Benjamin M. Rosen Bioengineering Center  
Photo credit: Christopher Michel for Caltech*



## 2024 High School Chemistry Olympiad

The **56th International Chemistry Olympiad** will be held July 21-30, 2024, in Riyadh Saudi Arabia. The US will send a team of 6 high school students (4 team members and 2 alternates) as well as mentors and coaches (see **2024 Team USA announcement on Chemistry Olympiad website**). They will compete in lab practical and written theoretical exams against teams from 80 different nations. The selection of US team members follows three steps: (1) a local qualifying exam, (2) a 3-part National exam (given locally), and (3) a weeklong study camp for the top 20 students.

Any interested US high school student can take the local qualifying exam. 284 students from the Silicon Valley ACS area took the local qualifying exam. These students came from over 35 high schools. We then nominate 14 students from our top scoring students to take the National exams. Although none of the students who took the National exams from our section were selected for study camp, we did have 3 students receive high honors and 6 students receive honors, which is a good showing and reflects high-quality chemical education. High honors are granted to the top 50 students in the country and honors recognize the top 200 students.

The high schools in the SVACS region with students selected to participate in the 2024

National exam were: Aragon High School (HS), Branham HS, Cupertino HS, The Harker School, Los Gatos HS, Lynbrook HS, Mountain View HS, Nueva HS, Palo Alto HS, Saratoga HS, St. Francis HS, and Valley Christian HS.

The students in our Section who were recognized for their excellent performance are:

**High Honors:** Neo Alpha, Harker; Yeonho Noh, Mountain View HS; Jianyu Wang, Lynbrook HS  
**Honors:** Advait Avadhanam, Saratoga HS; Forrest Chou, Palo Alto HS; Andrew Dong, Aragon HS; Siwen Luo, Lynbrook HS; Mihir Rane, St. Francis HS; Junhao Wang, Los Gatos HS

Sign-up for the 2025 exam will start in December. For more information, or to test yourself on one of the exams, go to <https://www.acs.org/education/students/highschool/olympiad.html>

For more information, please see:

- [U.S. National Chemistry Olympiad website](#)
- [About the International Chemistry Olympiad](#)
- [The 2024 U.S. National Chemistry Olympiad High Honors and Honors List](#)
- [2024 U.S. Chemistry Olympians named](#) (ACS News Release)
- Cottle, S. [2024 Team USA announced to participate in International Chemistry Olympiad](#), *C&EN*, June 18, 2024.



## The Materials Project

"Harnessing the power of supercomputing and state-of-the-art methods, the **Materials Project** provides open web-based access to computed information on known and predicted materials as well as powerful analysis tools to inspire and design novel materials.

The Materials Project is a multi-institution, multi-national effort to compute the properties of inorganic materials and to provide the data and associated analysis algorithms to materials researchers free of charge. The ultimate goal of the initiative is to reduce the time needed to invent new materials by focusing costly and time-consuming experiments on compounds that show promise computationally.

Supercomputing clusters at national laboratories provide the infrastructure that hosts The Materials Project computations, data, and algorithm, principally located at the Lawrence Berkeley National Laboratory's **NERSC** Scientific Computing Center and Computational Research Division and also at Oak Ridge's **OLCF** Argonne's **ALCF** and San Diego's **SDSC**."

[Learn more](#)

# CALENDAR OF EVENTS

<https://www.siliconvalleyacs.org/events/>

- July 2024 -

- Jul 8** **Summer STEAM at the Library: Chemistry**  
Sponsored by Friends of the Redwood City Public Library and Silicon Valley ACS  
3:30-5:30 pm, In person for grades 3-8, RCPL Downtown Location, 1044 Middlefield Road, Redwood City, Free, [Learn more](#)
- Jul 9** **Tech Trek**  
Sponsored by Silicon Valley ACS and American Association of University Women  
6:00-8:00 pm, In-person for 7th Grade Girls, Santa Clara University, [Learn more](#)
- Jul 10** **Crafting a Standout Grant Proposal: Tips and Success Stories**  
Professors Charlisa Daniels of Northern Kentucky University, Jodie Lutkenhaus of Texas A&M University, and Julian West of Rice University  
Sponsored by ACS Webinars and ACS Office of Grants Research  
11:00 am-Noon, Online, Free, [Registration required](#)
- Jul 13** **Silicon Valley ACS Annual Picnic and Awards**  
Cuesta Park Group BBQ Areas #1-2, Mountain View  
4:00-7:00 pm, Cost: \$10.00. Children: free. Pay with cash or check at the door. (Make checks out to "Silicon Valley ACS.")  
[Registration required by end of the day on July 10](#)
- Jul 17** **Résumé Development: Marketing Your Brand for an Industrial Chemistry Position**  
Adam Myers, ACS Career Consultant  
Sponsored by ACS Careers Office  
9:00-10:30 am, Online, Free, [Registration required](#)
- Jul 17** **How can ACS support your career as a Chemical Technical Professional?**  
Michelle Rivard, Dow, and Matthew Russell, Corteva Agrisciences  
Sponsored by ACS Webinars and ACS Committee on Technician Affairs  
11:00 am-Noon, Online, Free, [Registration required](#)
- Jul 18** **Python Scripting for Molecular Docking: Virtual Crash Course**  
Paul Craig, Ph.D. and Jessica Nash, Ph.D.  
Sponsored by Research Collaboratory for Structural Bioinformatics Protein Data Bank (RCSB PDB)  
10:00 am-2:00 pm, Online, Free, [Registration required](#)
- Jul 18** **A Different Way of Thinking: How Students Who are Neurodivergent can Flourish in Science**  
Maria Dulay, Stanford University; Prof. Christin Monroe, Landmark College; Holden Thorp, Editor-in-Chief, Science Family of Journals  
Sponsored by ACS Webinars, ACS Chemists with Disabilities Committee, and the ACS Office of Diversity, Equity, Inclusion & Respect  
11:00 am-Noon, Online, Free, [Registration required](#)
- Jul 24** **Avoiding IP Own Goals in Drug Discovery: Best Practices for Obtaining & Keeping Your IP**  
Eric Romeo and Olivia Uitto, IP attorneys and partners at Goodwin  
Sponsored by ACS Webinars and ACS Chemistry and the Law Division  
11:00 am-12:15 pm, Online, Free, [Registration required](#)
- Jul 24** **Healing Broken Hearts: Cardiovascular Implants**  
Subbu Venkatraman, Ph.D., Office of Innovation & Commercialization, UC San Diego, and Principal Investigator, iHealthTech, Singapore  
Sponsored by Golden Gate Polymer Forum (GGPF)  
5:00-6:00 pm, Online, Free/\$5 Donation, [Registration required by July 23rd at 1pm](#)
- Jul 25** **Bridging the Skills Gap Between the CHIPS and Science Act and Chemical Technical Professionals**  
Martha Ross, Brookings Metro, and John-David R. Rocha, ACS  
Sponsored by ACS Webinars and ACS Science Policy  
11:00 am-Noon, Online, Free, [Registration required](#)
- Jul 28** **Biennial Conference on Chemical Education (BCCE)**  
- Aug 1  
Sponsored by the ACS Division of Chemical Education (DivCHED)  
In person, University of Kentucky, Lexington, Kentucky, [Learn more](#)

- August 2024 -

- Aug 10** **Kid Makers: Pop Up Chemistry**  
Sponsored by Silicon Valley ACS and Redwood City Public Library (RCPL)  
2:00-3:00 pm, In person for ages 9-12, RCPL Downtown Location, 1044 Middlefield Road, Redwood City, Free, [Learn more](#)
- Aug 18-24** **ACS Fall 2024 Meeting**  
Denver, Colorado & Hybrid, [Registration and Housing are Open](#)



## Silicon Valley ACS Local Section Selected as a Finalist for Two ACS ChemLuminary Awards

*Below is the wonderful news we received from ACS President Mary Carroll about SVACS being a finalist for two ChemLuminary Awards. Descriptions of the activity that garnered the nominations for the two awards is provided below the letter.*



June 4, 2024

Dear Dr. Eberspacher, Chair of the Silicon Valley ACS,

On behalf of the American Chemical Society, I am delighted to inform you that the Silicon Valley Local Section has been selected as a finalist for the **ACS ChemLuminary Awards** in the following categories:

- Outstanding Local Section Career Program Award
- Outstanding NCW Event for a Specific Audience

The winners will be announced during the ACS Fall 2024 meeting in Denver. The ceremony takes place on Tuesday, August 20, in Plaza Ballroom A-C of the Sheraton Denver Downtown, and is open to all.

The event schedule is as follows:

- 8:00 pm - 9:00 pm: Poster Session & Reception
- 9:00 pm - 10:00 pm: ACS ChemLuminary Awards Ceremony
- 10:00 pm - midnight: Dance Social

The ceremony will feature a keynote address by **V. Michael Mautino**, retired from Covestro and the recipient of the 2024 Award for Volunteer Service to the American Chemical Society. The awards presentation given by 21 committees of the Society will follow. This year's theme is "**Elevating the Dedication of Our Volunteers**," which celebrates the work of volunteers to improve all people's lives through the transforming power of chemistry.

Congratulations on your outstanding achievements. We look forward to celebrating with you at the ACS ChemLuminary Awards ceremony!

Sincerely,

Mary K. Carroll, Ph.D., President, American Chemical Society

ACS ChemLuminary Awards | [chemluminary@acs.org](mailto:chemluminary@acs.org) | [www.acs.org/chemluminary](http://www.acs.org/chemluminary)

### SVACS activities nominated for recognition with a ChemLuminary Award

#### Outstanding Local Section Career Program Award

Paving the Path (PtP) was initiated as a peer mentorship program to support community college students interested in transferring to 4-year institutions. Activities of the PtP program include one-on-one peer mentoring, financial aid and college application seminars, and resume-building workshops. By far, the career panel proves to be most successful in engaging community college students in our section. In April 2023 we hosted a career panel tailored for this audience, composed of scientific professionals who all started their higher education journeys at community colleges. The panel was presented in hybrid format so students from a number of community colleges could attend without the hassle of Silicon Valley traffic.

On Thursday evening, April 27, 2023 over 50 community college students, alumni, instructors, and supporters from around our section gathered on Zoom for a Virtual Career Panel that showcased four scientists who started their higher education journeys at community colleges. Over the two-hour event, four wonderful panelists – industry professional Joel Bruegger, Associate Professor Kelly Chacón, Assistant Professor Andro Rios, and PhD student Victoria Tafuri – shared their stories and advice in a moderated panel, in an open Q&A session, and in small group breakout rooms.

Two special add-ons to this event included (1) an in-person watch party at Hartnell College where students gathered for SVACS-supplied pizza and to view the panel as a group and (2) a special raffle for ACS prizes for a couple of lucky winners who filled out our post-panel survey. Survey respondents said they would recommend the event to other people in the same stage of their education. Some feedback was that "This panel was very helpful and inspirational for a community college student like me." Other attendees mentioned "gaining wisdom from the panelists" as well as "now I have a better idea of possible career paths."

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A big take-home lesson for our section was the positive outcome of the watch party format, to serve as a model going forward. SVACS provided food and ACS swag for a Zoom watch party at an in-person gathering at Hartnell Community College in Salinas. Hartnell stepped up to host the event and SVACS members Steve Boyer and Jane Frommer stepped up to lead the in-person networking before and after the Zoomed panel. Going forward, SVACS plans to expand this in-person hybrid event with a watch party on each campus hosted by a faculty member paired with an SVACS member. With pizza, of course.

#### Outstanding NCW Event for a Specific Audience

The Silicon Valley local section embraced National Chemistry Week and conducted events at 4 different venues:

- Martin Luther King Library, San Jose, CA
- Salinas Community Science Center, Salinas, CA
- Ronald McDonald House, Palo Alto, CA
- Redwood City Library, Redwood City, CA

Over 300 students participated in hands-on experiments which encompassed some old favorites like Slime and Boo bubbles and some new experiments including "Cloudy with a Chance of Clear". Boo bubbles, which are made using dry ice, were a great way to attract attention from passers-by and draw them into the full event. In honor of the Halloween season, we incorporated iron filings in the slime mixture which made the slime more interactive and almost seem alive when a magnet was in proximity. We also had a medicinal plant experiment where the students were asked to match a sample of the medicinal plant with its essential oil, while learning about the natural origins of many of our medicines.

Ronald McDonald House is a facility where young outpatients and their families and siblings can stay while undergoing medical procedures at the Stanford Hospital. We made UV activated bead bracelets and played the board game that was included in the Celebrating Chemistry magazine.

At the Salinas Community Science Center, we explored the cochineal dye and water surface tension experiments.

Our section has an ongoing hands-on science program at the Redwood City Library, where we meet each month for an hour for a new science experiment. We have a regular following of students who come each month to try the new experiment. This is a particularly attractive program for homeschooled students who might not get as much exposure to science. For NCW, they evaluated the buffering capacity of magnesium hydroxide.

These events were supported by the chemistry clubs at San Jose State University and Santa Clara University, as well as volunteers from Silicon Valley local section. Who had more fun - the students or the volunteers? Each student left with a Mole Sticker, an ACS pencil, a tattoo or maybe even one of each!

The Silicon Valley section also participated in the NCW poetry contest. Several students submitted illustrated poems. The section awarded each participant a small gift card and submitted our favorite poem to the National contest. SVACS's Shreyas K was the ACS National 1st place winner in the Grade 6-8 category.

## ACS Funding and Award Opportunities

Deadlines July-September 2024

Name of Grant or Award	Recipient	Amount	Deadline
<i>Graduate Student and Postdoctoral Scholars Recognition Program</i>	Student	\$0, recognition	July 14, 2024
<i>Corporation Associates Seed Grant</i>	Industry, Chemistry Professional, Volunteer	Up to \$5,000	July 15, 2024
<i>Division Innovative Project Grants</i>	Industry, Chemistry Professional	Up to \$16,500 per year	July 15, 2024
<i>Corporation Associates Local Section &amp; International Chapter Grant</i>	Industry, Chemistry Professional, Volunteer, International	Up to \$1,000	July 15, 2024
<i>Trust in Science and Scientists Grant</i>	Industry, Chemistry Professional, Volunteer	\$1,500 - \$4,500	July 15, 2024
<i>Pfizer Emergent Leader Award</i>	Female/Female-Identified Student, Early Career	\$1,500	July 15, 2024
<i>Convergent Chemistry Communities Grant</i>	ACS Technical Divisions	Up to \$30,000 for activities occurring no more than two years after receiving the grant.	July 31, 2024
<i>CCS High School Chemical Safety Grant</i>	K-12 Teacher	Up to \$3,000	August 1, 2024
<i>Stanley C. Israel Regional Award for Advancing Diversity in the Chemical Sciences</i>	Industry, Institution, Faculty, Chemistry Professional	\$1,000 + Travel Reimbursement up to \$1500	August 1, 2024
<i>Latin American Women in Chemistry Awards</i>	International	\$2,000	August 4, 2024
<i>Teaching Green Fellowship</i>	Faculty	\$15,000 + travel	September 20, 2024
<i>Principal Investigator Development in Sustainability Grant</i>	Faculty	\$50,000	September 20, 2024
<i>Early Career Postdoctoral-Faculty Bridge Grant</i>	Faculty, Early Career	\$125,000	September 20, 2024
<i>Rising Stars in Green Chemistry Education Award</i>	Faculty, Early Career	\$1,000 + travel	September 20, 2024
<i>Career Achievement in Green Chemistry Education</i>	Faculty	\$5,000 + travel	September 20, 2024
<i>Science Café Mini-Grant</i>	Chemistry Professional, Volunteer	\$500	September 30, 2024



# Remaking the ACS National Meetings

Reimagining the must-attend events

## Future of Meetings Top Features



Creating **greater collaboration** in joint programming opportunities.



Providing **Hot or Late Breaking programming topics**.



Offering **fewer concurrent sessions**.



Presenting **more engaging topics and networking opportunities**.



Increasing **attendance and engagement** during sessions.



Increasing the number of **prominent distinguished speakers** from industry and academia.

## Redefine the ACS Meeting experience

### Future of Meetings Timeline

2024

- Convene Future of Meetings (FoM) Programming Workshop
- Launch Global Virtual Symposia as part of the digital experience (Spring)
- Pilot New Attendee Orientation and Sunday Networking event
- Pilot new half-day joint interdisciplinary sessions led by ACS Committee on Science
- Pilot new formats, including integrated poster sessions (Fall)

2025

- Roll-out of experimental program changes and evaluation
- Offer 3.5 days of technical sessions (Fall)
- Launch a multi-program operational approach
- Pilot new half-day interdisciplinary sessions led by ACS Committee on Science
- Pilot new industry-targeted solutions-based sessions (Fall)

For additional information, email  
[Futureofmeetings@acs.org](mailto:Futureofmeetings@acs.org)

## Making this Parkinson's Drug Is Just Turtles All the Way Down

A Reactions Science Video



[Watch Video on YouTube](#)

[Read Associated Article](#)

"L-DOPA is the best drug we have for Parkinson's disease, but its molecular mirror image, D-DOPA, causes dangerous side effects. Making L-DOPA without also making D-DOPA is surprisingly hard and requires a specific kind of molecule to pull off. But that specific molecule must be made from a different and equally specific molecule. In this video, our host George explains how one of the winners of the 2001 Nobel Prize in Chemistry pulled it off, and why "chiral synthesis," as it's called, is really just turtles all the way down."

Learn more about on-going ACS efforts to redefine large ACS meetings:

The Future of ACS Meetings: Comment by Amber S. Hinkle, Chair, Committee on Meetings and Expositions. *C&EN*, 2024, 102 (11), p 28, April 8, 2024

<https://pubs.acs.org/doi/10.1021/cen-10211-comment>

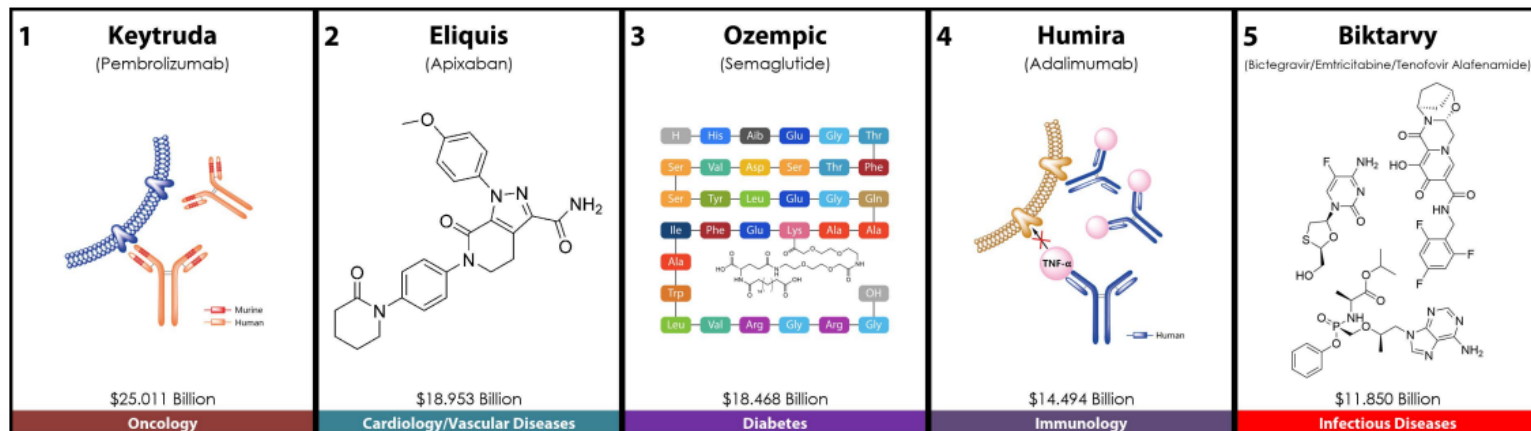
Future ACS Meetings & Expositions <https://www.acs.org/meetings/acs-meetings/future-meetings.html>

ACS Committee on Meetings and Expositions <https://www.acs.org/about/governance/committees/meetings-expositions.html>

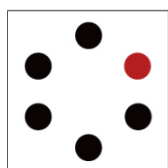
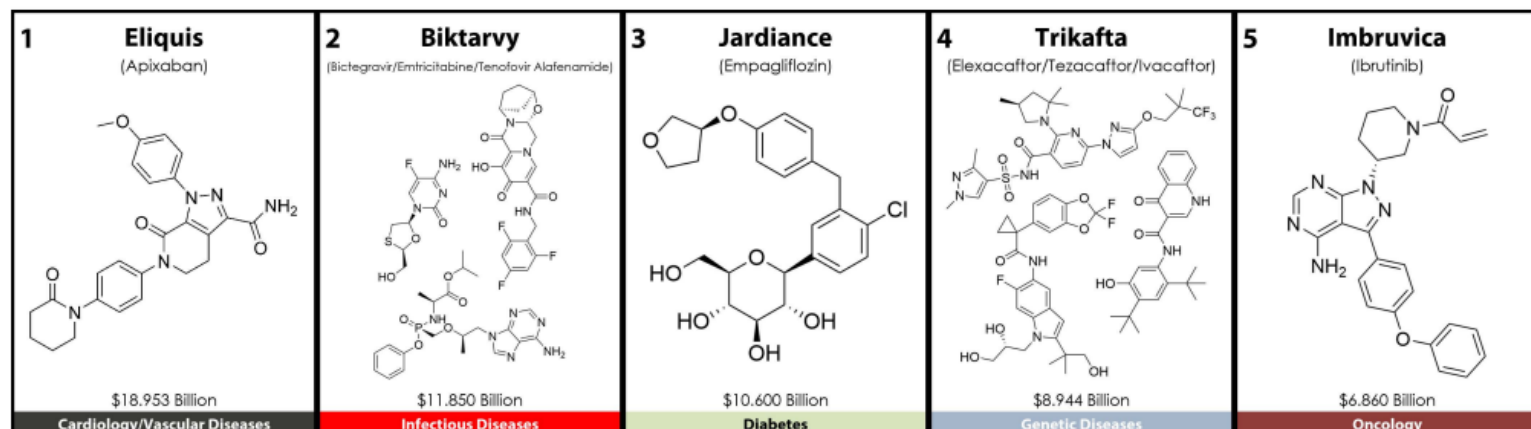
# Top 200 Drugs for 2023

**Chemistry Professor Jon Njardarson and his research group** at the University of Arizona have created since 2006 pharmaceutical posters that can be downloaded for free as high-resolution PDF files. **The posters** are part of their efforts to educate about how chemistry positively impacts our lives. Their attractive and accessible graphical summary helps communicate to the public and to researchers the critical role organic chemistry plays in the development of new medicines.

**Top 200 Drugs by Retail Sales in 2023** (PDF). Top 5 shown here. Click hyperlink to see all 200.  
Compiled and Produced by Ryan E. Williams and Hayden M. Leatherwood, Njardarson Group.



**Top 200 Small Molecule Drugs by Retail Sales in 2023** (PDF). Top 5 shown here. Click hyperlink to see all 200.  
Compiled and Produced by Ryan E. Williams and Hayden M. Leatherwood, Njardarson Group.



The  
Japan  
Institute  
of  
Heterocyclic  
Chemistry  
Publication



**HETEROCYCLES**

An International Journal for Reviews and Communications in Heterocyclic Chemistry

## Heterocycles – Open Access from CLOCKSS Archive

In November 2023, the Japan Institute for Heterocyclic Chemistry notified users that it was **suspending publication of Heterocycles** and removed all of the articles from their website. On June 24, 2024, access to Heterocycles was restored via **CLOCKSS**, a digital archiving service for academic publishers and research libraries. In a **news announcement** the next day, Dr. Alicia Wise, CLOCKSS' Executive Director, noted that they had "triggered" access to Heterocycles.

"In keeping with its unique mandate, CLOCKSS is proud to offer **continuing and public access to volumes 1-106 of Heterocycles**.

The trigger process involves coordination across multiple organizations, countries, and languages. It is ideally completed before content is removed from the web so that users can access the book or journal seamlessly. The process is not yet complete, but will be when the ~18,000 DOIs re-direct, thanks to the teams at CLOCKSS, Crossref,

and LOCKSS Program for collaborative efforts.

*Libraries, publishers, and all members of the scholarly community share a duty to preserve and protect knowledge for future generations."*



**CLOCKSS**

# Accelerating Drug Discovery

## Curated Dataset of Protein Structures from the Protein Data Bank with Predicted Hydrogen Positions Now Available

*This reprinted article by Michael Francis was posted on the Crystallographic Data Centre's Blog, June 18, 2024*

"Thanks to the combined computing power of Amazon Web Services (AWS) and Intel, the Cambridge Crystallographic Data Centre (CCDC) announced that a potentially significant advancement in drug discovery has been achieved. A curated data set of protein structures from the Protein Data Bank (PDB) with predicted hydrogen positions is now available for download. This project was supported by an Intel RISE Technology Initiative contribution.

Historically, collaborations with the pharmaceutical industry have enabled the development of reliable methods for interpreting interactions within protein binding sites using proprietary information not publicly available. Repeating these studies with PDB structures presented a challenge due to the absence of hydrogen positions in water networks within the proteins. Reliable predictions require databases of augmented protein structures where hydrogen positions are assigned.

Generating this information computationally is intensive, considering multiple possible models. Overcoming this computational challenge was possible for the CCDC through the combined

resources of Intel and AWS. The CCDC generated a comprehensive snapshot of protein cavities in the PDB, identifying potential binding sites for small molecules with accurately predicted hydrogen positions for all components.

Key Benefits

- **Accessibility:** This data set is freely available, enabling widespread use in drug discovery research and development and a commitment to FAIR data.
- **Efficiency:** By providing precomputed hydrogen positions, researchers save valuable time and resources, eliminating redundant computations.
- **Environmental Impact:** Reducing the necessity for repeated computations lowers the environmental footprint of large-scale computational tasks.

### Download the Protonated PDB Files

Researchers and developers in the field of drug discovery can [download the protonated PDB files from the CCDC download page](#). This initiative democratizes access to critical data, empowering scientific advancement regardless of access to extensive computational resources."

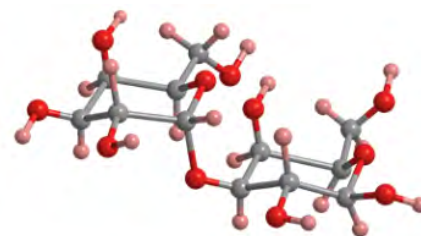
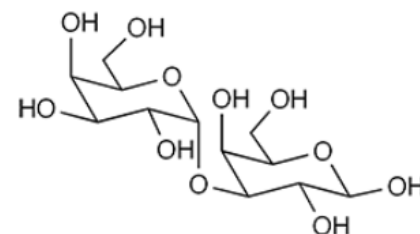
[Read more about this project on the AWS website](#)



CHEMISTRY

# Quiz

You don't have me in your body—and you want to keep it that way.  
What molecule am I?



Answer

## Updated Report to the U.S. Congress on Financing Mechanisms for Open Access Publishing of Federally Funded Research

"*This report* follows OSTP's report in November 2023 (November 2023 Report), which included an in-depth financial analysis of: (1) article processing charges (APCs) and transformative agreement costs borne by federal research grantees during fiscal years 2016 to 2021; (2) an assessment of these financing mechanisms on the volume of research publications authored by scientists from a variety of backgrounds and disciplines; and (3) a discussion of additional data needed to inform a more robust understanding of the financial impacts of public access policies for scholarly publications.

This current report elaborates on:

1. Implementation to advance federal public access policies. Updated agency public access policies will go into effect by December 31, 2025, in accordance with the 2022 Memorandum.
2. Trends in scholarly publishing since the release of the November 2023 Report, including further discussion of business models to enable public access to federally funded research, as well as domestic and global developments in advancing public access to research results.
3. An expansion of the analysis of estimated article processing charges paid to publish federally funded research from 2016 to 2022, with further discussion of limitations associated with calculating these charges.
4. Efforts to advance research integrity, including through implementation of federal public access policies and open science practices.
5. Continuing trends in peer review as they relate to research integrity, equity, and sustainability."

Learn more: <https://www.infodocket.com/2024/06/25/just-released-updated-report-to-the-u-s-congress-on-financing-mechanisms-for-open-access-publishing-of-federally-funded-research>



### UPDATED REPORT TO THE U.S. CONGRESS ON FINANCING MECHANISMS FOR OPEN ACCESS PUBLISHING OF FEDERALLY FUNDED RESEARCH

A Report by the  
WHITE HOUSE OFFICE OF SCIENCE AND TECHNOLOGY POLICY

JUNE 2024

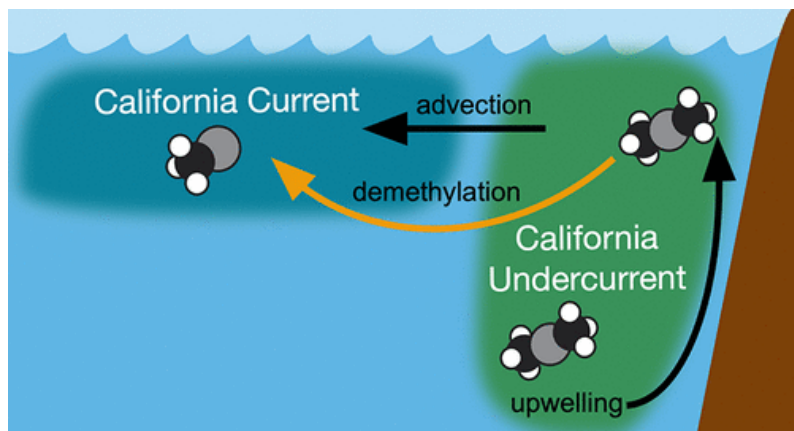


## Molecule of the Week Update: Dimethylmercury

**Dimethylmercury**<sup>1</sup> (Me<sub>2</sub>Hg) was the Molecule of the Week for *January 30, 2023*. It is an extremely neurotoxic compound that can be fatal if swallowed, inhaled, or absorbed through the skin. It is also highly flammable and suspected of causing cancer.

Me<sub>2</sub>Hg occurs in ocean waters and is responsible for the occurrence of mercury in seafood. Last month, Hannah M. Adams, Amina T. Schartup, and colleagues at the Universities of California at San Diego and Santa Cruz reported that *Me<sub>2</sub>Hg is a source of the methylmercury<sup>2</sup> cation* (MeHg<sup>+</sup>), the form of mercury found in marine life that is even more lethal than Me<sub>2</sub>Hg because it can cross the blood–brain barrier. The authors' findings from the ocean near the California coast challenge current understandings of the source of MeHg<sup>+</sup> that contend that the toxin is derived from inorganic mercury.

1. CAS Reg. No. 593-74-8
2. CAS Reg. No. 22967-92-6



## Welcome to the Silicon Valley Section of ACS



Each month, our Silicon Valley local ACS section receives a spreadsheet from national ACS with the names of members new to our section. The members are either new to ACS, have transferred in from other areas, or are the newest members - students. As a welcoming gesture, the SVACS Executive Committee offers new members free attendance at a catered SVACS event. Come join us at our in-person gatherings! To register as our guest for a catered event, [contact us](#) directly to receive complimentary admission for you and a friend. This month's picnic is one such opportunity to meet us. See page 1 for details.

We hope you will also join us for an outreach event, like judging a science fair, proctoring the high school Chemistry Olympiad or participating in a National Chemistry Week hands-on experiment event. The local section is a volunteer organization. Attend an event, volunteer to help, and get to know your local fellow chemists.

### New SVACS Members

Jiahua Deng  
Kathryn Kapp  
Adam Koble  
Anna Kolln  
Joseph Leet  
Laura Leibfried

Avi Mathur  
Carson Matier  
Thomas Mies  
N. Neil Ogimachi  
Kazuhito Saito

Katie Sanders  
Thea Schmit  
Dustin Scott Siegel  
Jiayue Wang  
Aileen Wu

## Patent Landscape Report on Generative Artificial Intelligence (GenAI) from the World Intellectual Property Organization (WIPO)

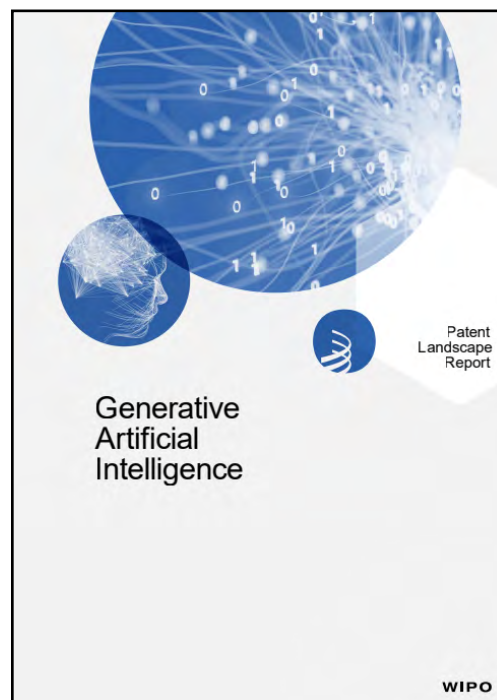
“Generative artificial intelligence (GenAI) is booming. It is a cutting-edge technology that is poised to disrupt economic, social, and cultural sectors, and it extends far beyond simple human-like text generation using chatbots. Drawing on original analysis of patent and scientific data, the WIPO patent landscape report on Generative AI provides a snapshot of the patent situation for GenAI.”

[Learn more](#)

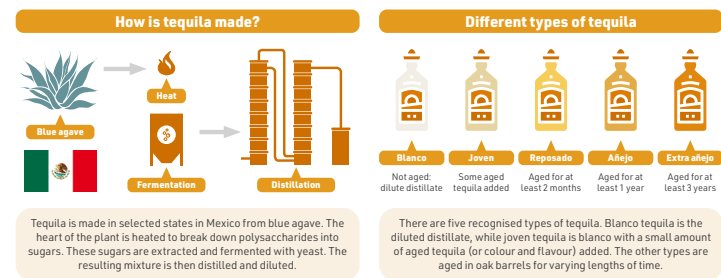
[Key Findings and Insights](#)

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About WIPO: The *World Intellectual Property Organization (WIPO)* leads the development of a balanced and effective global intellectual property ecosystem to promote innovation and creativity for a better and more sustainable future.



# The Chemistry of Tequila



**Blanco tequilas**

Hundreds of compounds have been identified in tequila. Some terpene compounds, such as those shown below, originate from the agave.

**α-terpineol**      **Linalool**

Many other compounds that contribute to tequila flavour are formed during fermentation or distillation. Some compounds that make important contributions are highlighted below.

**Ethyl hexanoate**      **Ethyl octanoate**  
**2-phenethyl acetate**      **2-phenethyl ethanol**  
**β-damascenone**      **Isoamyl alcohol**

**Aged tequilas**

Many of the compounds found in blanco tequilas also contribute to flavour in aged tequilas. However, additional compounds from the oak wood in which the tequila is aged are important flavour contributors.

**Ageing reactions**  
**Lignin hydrolysis**  
**Oxidation reactions**

**Vanillin**      **Eugenol**  
**Guaiacol**      **4-ethylguaiacol**

**Whisky lactones**

The above compounds are formed as the lignin in the wood breaks down and further oxidation reactions occur. Many of them are also found in other barrel-aged alcohols.

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Silicon Valley

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	2023-2025	Kristin Schmidt	2023-2025	Laura Yeager
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