CHEMWATCH

Bulletin Board

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ASIA PACIFIC

Australia has Published Mandatory Standards for Infant Products

2024-08-01

The first one is the Consumer Goods (Infant Sleep Products) Safety Standard 2024 which has a commencement date on 19 July 2024 and a transition period of 18 months. It replaces the current mandatory standards for folding cots and household cots, and also sets safety requirements for other infant sleep products.

The other one is the Consumer Goods (Infant Products) Information Standard 2024 which has a commencement date on 19 January 2026. This standard sets new labeling requirements for infant products.

The Consumer Goods (Infant Sleep Products) Safety Standard 2024 applies to Infant Sleeping Product with the following definition:

Infant Sleep Product:

1. means a product that:

- is designed, intended, marketed, supplied, or offered for supply, for use as a sleeping facility for an infant or for use as a facility to soothe or settle an infant; and
- has a surface on which an infant may lay; and
  includes a product that is designed to convert to an infant sleep product.
  This standard sets safety requirements for folding cots, household cots, bassinets and other infant sleep products as listed in the table below

Read More

Bureau Veritas, 01-08-24

https://www.cps.bureauveritas.com/newsroom/australia-has-published-mandatory-standards-infant-products

FSANZ to advance nutrition labelling with a focus on consumers

2024-08-13

Food Standards Australia New Zealand (FSANZ) is set to progress a package of work on nutrition labelling standards to better support consumers to make informed and healthy dietary choices.

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Australian and New Zealand food ministers recently agreed to FSANZ scoping work to improve front- and back-of-pack nutrition information labelling and finalising alcohol labelling proposals.

FSANZ will begin preparatory work to support mandating the front-of-pack Health Star Rating (HSR) system should industry not meet voluntary uptake targets. The work will inform future decisions by food ministers on the HSR and support efficient implementation if the system is mandated.

HSR work will be undertaken in parallel with scoping of a holistic review of the nutrition information panel (NIP) found on the back of packaged foods. Any review would be the first for the NIP in over 20 years, supporting optimised nutrition information labelling for consumers.

FSANZ will advance work on two alcohol labelling proposals while undertaking HSR and NIP review scoping activities.

Proposal P1059 – Energy labelling on alcoholic beverages is examining options for the declaration of energy content information in a prescribed format on the label of packaged alcoholic beverages. If approved, the labelling will allow consumers to compare the kilojoule content of alcoholic beverages, just like they can for food products.

Proposal P1049 – Carbohydrate and sugar claims on alcoholic beverages seeks to clarify existing Food Standards Code permissions for nutrition content claims about carbohydrate and sugar on alcohol.

Read More

FSANZ, 13-08-24

https://www.foodstandards.gov.au/media/fsanz-advance-nutrition-labelling-focus-consumers

AMERICA

New Jersey Bill Seeks to Regulate THC-Infused Drinks That Are 'Legal' Today

2024-08-18

Heads up, New Jersey! A new bill is making waves in the Garden State, and it could soon change the game for THC-infused drinks. If you've been enjoying these beverages legally, things might be about to shift in a big way.

The bill aims to regulate the production and sale of "intoxicating hemp products," specifically targeting those with THC concentrations over 0.5 milligrams per serving or 2.5 milligrams per package. Essentially, if your drink packs more of a punch than these limits, it could be banned from the shelves.

Here's a quick rundown of what this bill means:

Definition of Intoxicating Hemp Products: Any hemp product with a THC concentration exceeding the stated limits falls under this new regulation.

Licensing Requirements: Sellers of these potent products will need a license from the Cannabis Regulatory Commission or a specific liquor license.

Prohibited Sales: The bill prohibits the sale of hemp products or cannabis items that aren't derived from naturally occurring, biologically active chemical constituents.

Regulations and Penalties: The Cannabis Regulatory Commission will be in charge of setting rules on packaging, labeling, product testing, and THC amounts. Violators could face civil penalties and product confiscation.

Local Taxes: Intoxicating hemp beverages sold by liquor license holders will be subject to local taxes, with the revenue going to the Cannabis Regulatory, Enforcement Assistance, and Marketplace Modernization Fund.

Read More

Shore News, 18-08-24

https://www.shorenewsnetwork.com/2024/08/18/new-jersey-bill-seeks-to-ban-thc-infused-drinks-that-are-legal-today/

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EPA Science Advisors Confirm Foundational Flaws in Formaldehyde TSCA Risk Evaluation and IRIS Assessment

2024-08-05

The American Chemistry Council's (ACC) Formaldehyde Panel issued the following statement on the Scientific Advisory Committee on Chemicals (SACC) report on the Environmental Protection Agency's (EPA) Draft Toxic Substances Control Act (TSCA) Risk Evaluation for formaldehyde, which is based on a 2022 draft assessment under EPA's Integrated Risk Information System (IRIS):

The report highlights fundamental flaws that demonstrate that the draft risk evaluation fails to meet TSCA's scientific standards and process requirements. EPA's peer reviewers echoed important concerns we have previously raised, including the failure to incorporate dozens of high-quality studies as well as assessments by authoritative bodies like the World Health Organization and European Union, that have been raised by other peer reviewers, scientific experts, and the public for over a decade.

The SACC peer reviewers found that the TSCA program's reliance on a draft IRIS assessment inappropriate, in particular the report stated:

On chronic noncancer endpoints: "Concerns were raised by some Committee members regarding studies selected by ORD IRIS for chronic non-cancer hazards. These studies are mainly observational and unreliable for identifying a point of departure. The studies identified by ORD IRIS for the weight of evidence for chronic human health non-cancer hazard do not adequately address the chosen endpoint."

On cancer endpoints: "Many Committee members recommended not using the IUR published in the 2022 Draft Formaldehyde IRIS assessment" with these members recommending use of "a mode of action approach where there is a threshold concentration below which no cancer is anticipated."

Read More

American Chemistry Council, 05-08-24

https://www.americanchemistry.com/chemistry-in-america/news-trends/press-release/2024/epa-science-advisors-confirm-foundational-flaws-in-formaldehyde-tsca-risk-evaluation-and-iris-assessment

Back to School Safety: How Disinfectants Help Ensure a Healthy Environment for Students

2024-08-06

The beginning of the school year is a time of excitement, but it can also bring worries about the potential spread of sickness. Schools are high-traffic areas where students, teachers, and staff work in close proximity. This increased interaction and shared spaces can create an ideal environment for the transmission of various viruses and bacteria. From common colds to more serious outbreaks, the risk of illness can disrupt the learning process, affect attendance, and pose a significant challenge to maintaining a healthy school community.

Effectively Using Disinfectants and Sanitizers to Help Control Germs

A disinfectant is used to help kill disease-causing pathogens (such as bacteria, viruses, and fungi) on hard surfaces and in water. Sanitizers are used to lower the number of pathogens on surfaces to a safe level. Unlike soap and regular cleaning products, disinfectants and sanitizers are registered by the U.S. Environmental Protection Agency (EPA), which evaluates data on each product to ensure that they pose no unreasonable risk to human health and the environment and data showing that they help kill or control the different pathogens listed on the product label (e.g., e. coli, types of flu-causing viruses). School employees can choose the product needed to slow the transmission of any known illnesses circulating in the school by carefully reviewing the labels of EPA-registered disinfectants and sanitizers.

Read More

American Chemistry Council, 06-08-24

https://www.americanchemistry.com/chemistry-in-america/news-trends/blog-post/2024/back-to-school-safety-how-disinfectants-help-ensure-a-healthy-environment-for-students

The Ongoing Battle Against Underground Storage Tank Leaks

2024-06-10

Owning and operating an underground storage tank (UST) involves serious practical and legal responsibilities. These systems have the potential to leak, often going unnoticed for long periods, resulting in severe environmental damage and costly clean-ups. Understanding

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the common causes of UST leaks and having the proper detection mechanisms in place is essential for safety and compliance.

Recent incidents highlight the ongoing risk and impact of underground storage tank (UST) leaks. Earlier this year, the state of Washington found a Chevron Station owner liable in a gas leak. In the past week, a petroleum spill at a Porter County, Indiana truck stop and a significant gasoline leak/explosion in Broward County, Florida underscore the critical need for vigilant management and maintenance of these systems.

Read More

Environment + Energy Leader, 10-06-24

https://www.environmentenergyleader.com/2024/06/the-ongoing-battle-against-underground-storage-tank-leaks/

8 ways to avoid giving your kids food with artificial coloring

2024-08-05

It's no secret kids love bright colors. Just look at the snack aisle in the grocery store, lined with vividly packaged products marketed to children and teens.

But the source of the often eye-poppingly bright food inside the packaging may be toxic artificial food coloring.

Chemicals marketed to kids and teens

Many foods marketed to kids contain artificial food dye, including such snack mainstays as flavored yogurt, applesauce and fruit cups, chips and crackers, trail mix, packaged baked goods containing fruit, and granola and protein bars.

It doesn't help that these foods are also typically high in sweeteners, salt and fat.

In one study, researchers found nearly all candy and fruit-flavored snacks contained artificial dye. Across all food categories, it could be found in nearly two in five products in the store the study analyzed. Only fresh produce did not contain artificial food dye.

California's environmental health agency has said consumption of these chemicals "can result in" behavioral problems in children, including

hyperactivity. Kids' developing bodies make them especially vulnerable to food dye exposure.

A wide range of brands and fast food chains have begun to phase out artificial colors, according to ingredients labels and news releases. But the chemicals are still found in many products on supermarket shelves, including many you'd never suspect were colored artificially.

Last year, a bill banning Red Dye No. 3 in California was signed into law. Now another bill has passed the state Assembly and is up for debate in the Senate. It would ban public schools in the state from serving foods containing any of six commonly used artificial colors.

Even with these positive developments, parents and caregivers who want to help their kids avoid artificial food dye may find themselves swimming upstream.

Read More

EWG, 05-08-24

https://www.ewg.org/news-insights/news/2024/08/8-ways-avoid-giving-your-kids-food-artificial-coloring

EUROPE

Notifying exports of PIC chemicals for 2025

HSE, the GB PIC Designated National Authority (DNA), is inviting companies to submit notifications for exports of chemicals in the GB PIC list that are expected to take place during 2025.

2024-08-19

The GB PIC Regulation requires the first export of a listed chemical in any calendar year, to any country, to be notified to the DNA at least 35 days before the intended date of export. Export includes the movement of a listed chemical from GB to Northern Ireland (NI).

Early notification ensures HSE has sufficient time to process notifications and seek the explicit consent of the importing country, where required, or to consider evidence for the granting of a waiver where there is no response to repeated requests for consent.

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What you need to do?

Export notifications

- Complete a GB PIC export notification form. You can find information on the notification processon HSE's PIC website, as well as supporting guidance on how to complete the form
- Send completed forms to ukdna@hse.gov.uk
- Include the following details in the subject line of your email:

GB PIC - notification - company name - chemical/mixture - importing country name – 2025

- When submitting your export notifications, attach only one export notification form and accompanying safety data sheet (SDS) to each email
- In addition to an SDS in English, provide an SDS in the official language of the importing country, if available, or in one of its principal languages. If you do not attach an SDS, sections 4 and 5 of the form become mandatory

Read More

UK HSE, 19-08-24

https://www.hse.gov.uk/index.htm

Celebrating International Youth Day: Empowering young adults for a sustainable future

2024-08-12

Today is International Youth Day, a special day that celebrates the important role young people play in driving societal change and development. This year, our members have been busy with projects and initiatives focused on empowering young adults through innovative projects that emphasise sustainability, climate action, and social inclusion.

The Spark project: Climate action through youth engagement

The Spark project stands out as a beacon of youth engagement in climate action. It aimed to elevate awareness about the multifaceted impacts of climate change and inspire young citizens to become proactive climate activists. This project saw ZERO, our Portuguese member, join forces with 19 other organisations from 12 EU Member States and the UK.

Throughout its duration, the Spark project reached over 25,000 young people in Portugal alone, with its influence spreading to more than 2 million across Europe. Key materials (in Portuguese) developed during the project, including an engaging project page, an informative quiz, and a comprehensive activism guide, continue to serve as valuable resources for young climate enthusiasts. These tools not only educate but also empower the youth to take meaningful action against climate change.

Read More

Zero Waste Europe, 12-08-24

https://zerowasteeurope.eu/2024/08/celebrating-international-youth-day-empowering-young-adults-for-a-sustainable-future/

INTERNATIONAL

Mercury has long poisoned gold miners. This new strategy is helping change that

2024-08-15

In the small coastal town of Guapi, Colombia, Mary Luz Ante Orobio is meeting with a group she calls "the unstoppable women."

They are gathered around a wooden chest filled with loose cash, a ledger and a calculator. Orobio flips through the ledger, eyes poring over tidy notes outlining a series of financial investments. She jots down some numbers before distributing cash among the group.

The women are members of one of 80 local savings and credit groups in Colombia formed with the help of planetGOLD, a programme led by the United Nations Environment Programme (UNEP). These groups provide rural communities dependent on small-scale gold mining with new financing opportunities, allowing them to invest in technology and tools to reduce reliance on mercury. This toxic chemical has been used in small-scale gold mining for more than 3,000 years and can cause irreversible brain damage.

"There is a lot of illegal mining around here. We want to counteract that, because it is polluting the environment," says Orobio. "From the savings, women can [upgrade] their sluice boxes, can get their [sluice box] rugs... This group allows women to create their own small businesses and be [independent] from money or resources that the men bring home."

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Read More

UNEP, 15-08-24

https://www.unep.org/news-and-stories/story/mercury-has-long-poisoned-gold-miners-new-strategy-helping-change

EU-Mercosur to meet in September signaling movement in trade talks

2024-08-08

European Union and South American negotiators will meet on Sept. 4-6 in Brasilia in the first in-person talks since April, raising hopes an EU-Mercosur trade deal can be concluded this year, diplomats said.

In the works for two decades, an agreement has been delayed by European concerns over environmental safeguards and complaints by the Mercosur trade bloc that those questions are motivated by protectionism.

"We are traveling to Brasilia for an in-person round of negotiations 4-6 September," a European diplomat said. "The end-of-year timetable for conclusion is realistic," he said.

Brazil and Uruguay both confirmed the dates of the meeting.

Uruguay's foreign ministry said that the negotiating process "continues firmly" and that technical work has carried on "uninterrupted" between both sides.

"There is interest from Mercosur in closing this agreement," a Uruguayan foreign ministry spokesperson told Reuters on Wednesday.

Read More

Reuters, 08-08-24

https://www.reuters.com/world/europe/eu-mercosur-meet-september-signaling-movement-trade-talks-2024-08-07/

REACH Update

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Have your say in our consultations

2024-08-23

Contribute to chemical safety in the EU by submitting your input on our topical consultations and calls for evidence.

This week, we have launched two new consultations on harmonised classification and labelling proposals for:

- 4-hydroxy-4-methylpentan-2-one; diacetone alcohol (EC 204-626-7, CAS 123-42-2); and
- 8-methyldecan-2-yl propionate; 8-methyldecan-2-yl propanoate (EC -, CAS 81931-28-4).

Have your say until 18 October 2024.

Check also other open consultations on our website:

- Applications for authorisation;
- Testing proposals;
- Potential candidates for substitution and on derogations conditions of biocidal products; and
- Occupational exposure limits.

Read More

ECHA, 23-08-24

https://echa.europa.eu/consultations/current

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Janet's Corner

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Producer Humor

2024-08-30

https://au.pinterest.com/pin/149111437635650896/

Benzidine

2024-08-30

USES [2,3]

In the past, industry used large amounts of benzidine to produce dyes for cloth, paper, and leather. However, it has not been made for sale in the United States since the mid-1970s. Major U.S. dye companies no longer make benzidine-based dyes. Benzidine is no longer used in medical laboratories or in the rubber and plastics industries. However, small amounts of benzidine may still be manufactured or imported for scientific research in laboratories or for other specialised uses. Some benzidine-based dyes (or products dyed with them) may also still be brought into the United States.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

The general population is not likely to be exposed to benzidine through contaminated air, water, soil, or food. Benzidine is a manufactured chemical that does not occur naturally in the environment. Currently, the United States industry makes and uses very little (if any) benzidine, and no releases to air, water, or soil are reported on the Toxic Release Inventory (TRI). Only rarely has benzidine been detected in areas other than waste sites, and it has not been found in food. Some dyes used to colour foods or drinks may contain impurities that can be broken down to benzidine once inside the body. If you live near a hazardous waste site, you could be exposed to benzidine by drinking contaminated water or by breathing or swallowing contaminated dust and soil. Benzidine can also enter the body by passing through the skin. Some quantities of dyes made from benzidine may still be brought into the United States. These may contain small amounts of benzidine as a contaminant, or chemicals that may be broken down in the body to benzidine. If you use such dyes to dye paper, cloth, leather, or other materials, you may be exposed by breathing or swallowing dust, or through skin contact with dust. You may be exposed in a similar way if you work at or near hazardous waste sites.

Routes of Exposure

Benzidine can enter your body if you breathe air that has small particles of benzidine or dust to which benzidine is attached. It can also enter your body if you drink water or eat food that has become contaminated

Benzidine, (4,4'-di-aminobiphenyl), is the solid organic compound with the formula (C6H4NH2)2. [1] It is a manu-factured chemical that does not occur naturally. Benzidine is a crystalline (sandy or sugar-like) solid that may be greyish-yellow, white, or reddish-grey. It will evaporate slowly from water and soil. Its flammability, smell, and taste have not been described. In the environment, benzidine is found in either its "free" state (as an organic base), or as a salt (for example, benzidine dihydrochloride or benzidine sulphate). In air, benzidine is found attached to

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with benzidine. If your skin comes in contact with benzidine, it could also enter your body. Generally, it will take only a few hours for most of the benzidine to get into your body through the lungs and intestines. It may take several days for most of the benzidine to pass through your skin. Breathing, eating, or drinking benzidine-based dyes may also expose you to benzidine. Your intestines contain bacteria that can break down these dyes into benzidine. Once in your body, only a small portion of benzidine will leave as waste in your urine and feces. Your body will change most of the benzidine into many different chemical forms (called metabolites), which dissolve readily in your bodily fluids and are easy for your body to remove. Some of these changed forms of benzidine appear to cause many of the chemical's harmful effects. Studies show that after benzidine has entered your body, most of it (and its changed forms) will be removed within a week.

HEALTH EFFECTS [4]

Acute Health Effects

No information is available on the acute effects of benzidine in humans via inhalation exposure. Benzidine is considered to be very acutely toxic to humans by ingestion. Symptoms of acute ingestion exposure include cyanosis, headache, mental confusion, nausea, and vertigo. Dermal exposure may cause skin rashes and irritation. Tests involving acute exposure of rats and mice have shown benzidine to have high toxicity from oral exposure.

Carcinogenicity

Numerous epidemiologic studies have demonstrated occupational exposure to benzidine to result in an increased risk of bladder cancer.

Animal studies have reported various tumour types at multiple sites from benzidine exposure via oral, inhalation, and injection exposure.

EPA has classified benzidine as a Group A, human carcinogen.

Other Effects

Chronic exposure to benzidine in humans may result in bladder injury. The Reference Dose (RfD) for benzidine is 0.003 milligram per kilogram body weight per day (mg/kg/d) based on brain cell vacuolisation in mice and liver cell alterations in female mice. The California Environmental Protection Agency (CalEPA) has established a chronic reference exposure

level of 0.01 milligrams per cubic metre (mg/m3) for benzidine based on neurological, liver, and spleen effects in mice.

SAFETY

First Aid Measures [5]

- **Eye Contact:** Check for and remove any contact lenses. In case of contact, immediately flush eyes with plenty of water for at least 15 minutes. Get medical attention.
- **Skin Contact:** In case of contact, immediately flush skin with plenty of water. Cover the irritated skin with an emollient. Remove contaminated clothing and shoes. Wash clothing before reuse. Thoroughly clean shoes before reuse. Get medical attention.
- **Serious Skin Contact:** Wash with a disinfectant soap and cover the contaminated skin with an anti-bacterial cream. Seek medical attention.
- **Inhalation:** If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention.
- **Ingestion:** Do NOT induce vomiting unless directed to do so by medical personnel. Never give anything by mouth to an unconscious person. If large quantities of this material are swallowed, call a physician immediately. Loosen tight clothing such as a collar, tie, belt or waistband.

Workplace Controls & Practices [4]

Control measures include:

Use process enclosures, local exhaust ventilation, or other engineering controls to keep airborne levels below recommended exposure limits. If user operations generate dust, fume or mist, use ventilation to keep exposure to airborne contaminants below the exposure limit.

Personal Protective Equipment [5]

The following personal protective equipment is recommended when handling benzidine:

- Splash goggles;
- lab coat;
- dust respirator (be sure to use an approved/certified respirator or equivalent); and

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- gloves.

Personal Protection in Case of a Large Spill:

- Splash goggles;
- full suit;
- dust respirator;
- boots; and
- gloves.
- A self-contained breathing apparatus should be used to avoid inhalation of the product.

REGULATION

United States

OSHA: The Occupational Safety & Health Administration has set the following Permissible Exposure Limit (PEL) for benzidine:

- General Industry: 29 CFR 1910.1010 requirements identical to 29 CFR 1910.1003 - 13 Carcinogens (4-Nitrobiphenyl, etc.) -- Cancer-Suspect Agent
- Construction Industry: 29 CFR 1926.1110 requirements identical to 29 CFR 1910.1003 - 13 Carcinogens (4-Nitrobiphenyl, etc.) -- Cancer-Suspect Agent
- Maritime: 29 CFR 1915.1010 requirements identical to 29 CFR 1910.1003 - 13 Carcinogens (4-Nitrobiphenyl, etc.) -- Cancer-Suspect Agent

ACGIH: The American Conference of Governmental Industrial Hygienists has set the following threshold Limit Value (TLV) for benzidine: Exposure by all routes should be carefully controlled to levels as low as possible; Skin; Appendix A1 - Confirmed Human Carcinogen

NIOSH: The National Institute for Occupational Safety and Health has set the following Recommended Exposure Limit (REL): Appendix A - NIOSH Potential Occupational Carcinogens; Appendix C - Supplementary Exposure Limits

REFERENCES

1. http://en.wikipedia.org/wiki/Benzidine
2. http://www.atsdr.cdc.gov/phs/phs.asp?id=567&tid=105

3. http://www.epa.gov/ttn/atw/hlthef/benzidin.html
4. http://www.sciencelab.com/msds.php?msdsId=9923046

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First lung cancer vaccine given to patient in international trial

2024-08-29

A 67-year-old London man with lung cancer has been the first to receive a new cancer vaccine as part of an international trial. The early-stage research will test the immune therapy's safety and whether it can be used together with existing cancer treatments.

When you hear 'vaccine,' you probably think of the jab for the flu or COVID-19. However, a vaccine is any substance that helps the body's immune system recognize and fight diseases, including cancer.

A 67-year-old lung cancer patient from London has been the first recipient of a new investigational cancer vaccine at the National Health Service (NHS) University College London Hospitals (UCLH).

"Lung cancer remains the leading cause of cancer deaths worldwide, with an estimated 1.8 million deaths in 2020," said Siow Ming Lee, professor of medical oncology at University Hospital London and leader of the UK arm of the study. "We are now entering this very exciting era of mRNA-based immunotherapy clinical trials to investigate the treatment of lung cancer … We hope this will provide an opportunity to further improve outcomes for our NSCLC [non-small cell lung cancer] patients, whether in the early or advanced stages."

Non-small cell lung cancer, or NSCLC, is one of two primary kinds of lung cancer and is the most common kind. The other kind is small cell lung cancer (SCLC). In NSCLC, cancer cells originate in the lung tissue, and although it grows slower than the small cell variant, NSCLC has often spread to other body parts by the time it's diagnosed.

The novel vaccine, BNT116, made by the German biotech company BioNTech, uses messenger RNA (mRNA) to present markers from the tumor to the patient's immune system so it can recognize and fight the cancer cells carrying the tumor markers. The vaccine works selectively on cancer cells via the patient's immune system, rather than, say, chemotherapy, which can be toxic to both cancerous and healthy cells.

"The strength of the approach we are taking is that the treatment is aimed at being highly targeted towards cancer cells," said Dr Sarah Benafif, who's leading the trial.

About 130 participants will be enrolled in the study across seven countries. Patients at different stages of NSCLC, from those in the early stage before treatment with surgery or radiation therapy to those with late-stage

or recurrent cancer. This early-stage research will determine whether BNT116 is safe and well-tolerated as a standalone anti-tumor treatment and whether it works synergistically when it's given alongside established NSCLC treatments.

Janusz Racz is the trial's first participant. As someone who works in a scientific field, he is glad to be able to contribute to the advancement of cancer treatment.

"I thought it over, and … decided to take part because I hope it will provide a defense against cancer cells," Racz said. "But I also thought that my participation in this research could help other people in future and help this therapy become more widely available.

"As a scientist myself, I know that science can only advance if people agree to participate in programs like this," continued Racz."I work in artificial intelligence, and I am open to trying new things. My family did research about the trial, too, and they supported me taking part."

Source: UCLH/NHS

New Atlas, 29 August 2024

https://newatlas.com

AI Cracks the Chemistry Code to Better, Longer-lasting Solar Panels

2024-08-28

Their novel approach involved AI-driven closed-loop experimentation and automated chemical synthesis to uncover the underlying chemical principles of stability, offering fresh insights into molecular design for organic solar cells.

Artificial intelligence is a powerful tool for researchers, but with a significant limitation: The inability to explain how it came to its decisions, a problem known as the "AI black box." By combining AI with automated chemical synthesis and experimental validation, an interdisciplinary team of researchers at the University of Illinois Urbana-Champaign has opened up the black box to find the chemical principles that AI relied on to improve molecules for harvesting solar energy.

Advancements in Light-Harvesting Molecule Stability

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The result produced light-harvesting molecules four times more stable than the starting point, as well as crucial new insights into what makes them stable — a chemical question that has stymied materials development.

The interdisciplinary team of researchers was co-led by U. of I. chemistry professor Martin Burke, chemical and biomolecular engineering professor Ying Diao, chemistry professor Nicholas Jackson and materials science and engineering professor Charles Schroeder, in collaboration with along with University of Toronto chemistry professor Alán Aspuru-Guzik. They published their results today (August 28) in the journal Nature.

"New AI tools have incredible power. But if you try to open the hood and understand what they're doing, you're usually left with nothing of use," Jackson said. "For chemistry, this can be very frustrating. AI can help us optimize a molecule, but it can't tell us why that's the optimum — what are the important properties, structures and functions? Through our process, we identified what gives these molecules greater photostability. We turned the AI black box into a transparent glass globe."

Solving Photostability With Closed-Loop Experimentation

The researchers were motivated by the question of how to improve organic solar cells, which are based on thin, flexible materials, as opposed to the rigid, heavy, silicon-based panels that now dot rooftops and fields.

"What has been hindering commercialization of organic photovoltaics is problems with stability. High-performance materials degrade when exposed to light, which is not what you want in a solar cell," said Diao. "They can be made and installed in ways not possible with silicon and can convert heat and infrared light to energy as well, but the stability has been a problem since the 1980s."

Accelerating Discovery with Modular Chemistry and AI

The Illinois method, called "closed-loop transfer," begins with an AI-guided optimization protocol called closed-loop experimentation. The researchers asked the AI to optimize the photostability of light-harvesting molecules, Schroeder said. The AI algorithm provided suggestions about what kinds of chemicals to synthesize and explore in multiple rounds of closed-loop synthesis and experimental characterization. After each round, the new data were incorporated back into the model, which then provided improved suggestions, with each round moving closer to the desired outcome.

The researchers produced 30 new chemical candidates over five rounds of closed-loop experimentation, thanks to building block-like chemistry and automated synthesis pioneered by Burke's group. The work was done at the Molecule Maker Lab housed in the Beckman Institute for Advanced Science and Technology at the U. of I.

"The modular chemistry approach beautifully complements the closed-loop experiment. The AI algorithm requests new data with maximized learning potential, and the automated molecule synthesis platform can generate the new required compounds very quickly. Those compounds are then tested, the data goes back into the model, and the model gets smarter — again and again," said Burke, who also is a professor in the Carle Illinois College of Medicine. "Until now, we've been largely focused on structure. Our automated modular synthesis now has graduated to the realm of exploring function."

Unveiling the Secrets of Molecular Stability

Instead of simply ending the query with the final products singled out by the AI, as in a typical AI-led campaign, the closed-loop transfer process further sought to uncover the hidden rules that made the new molecules more stable.

As the closed-loop experiment ran, another set of algorithms was continuously looking at the molecules made, developing models of chemical features predictive of stability in light, Jackson said. Once the experiment concluded, the models provided new lab-testable hypotheses.

"We're using AI to generate hypotheses that we can validate to then spark new human-driven campaigns of discovery," Jackson said. "Now that we have some physical descriptors of what makes molecules photostable, that makes the screening process for new chemical candidates dramatically simpler than blindly searching around chemical space."

To test their hypothesis about photostability, the researchers investigated three structurally different light-harvesting molecules with the chemical property they identified — a particular high-energy region — and confirmed that choosing the proper solvents made the molecules up to four times more light-stable.

"This is a proof of principle for what can be done. We're confident we can address other material systems, and the possibilities are only limited by our imagination. Eventually, we envision an interface where researchers can input a chemical function they want and the AI will generate

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hypotheses to test," Schroeder said. "This work could only happen with a multidisciplinary team, and the people, resources, and facilities we have at Illinois, and our collaborator in Toronto. Five groups came together to generate new scientific insight that would not have been possible with any one of the sub-teams working in isolation."

Sci Tech Daily, 28 August 2024

https://scitechdaily.com

Catalytic process vaporizes plastic bags and bottles, yielding gases to make new, recycled plastics

2024-08-29

A new chemical process can essentially vaporize plastics that dominate the waste stream today and turn them into hydrocarbon building blocks for new plastics.

The catalytic process, developed at the University of California, Berkeley, works equally well with the two dominant types of post-consumer plastic waste: polyethylene, the component of most single-use plastic bags; and polypropylene, the stuff of hard plastics, from microwavable dishes to luggage. It also efficiently degrades a mix of these types of plastics.

The process, if scaled up, could help bring about a circular economy for many throwaway plastics, with the plastic waste converted back into the monomers used to make polymers, thereby reducing the fossil fuels used to make new plastics. Clear plastic water bottles made of polyethylene tetraphthalate (PET), a polyester, were designed in the 1980s to be recycled this way. But the volume of polyester plastics is minuscule compared to that of polyethylene and polypropylene plastics, referred to as polyolefins.

"We have an enormous amount of polyethylene and polypropylene in everyday objects, from lunch bags to laundry soap bottles to milk jugs—so much of what's around us is made of these polyolefins," said John Hartwig, a UC Berkeley professor of chemistry who led the research.

"What we can now do, in principle, is take those objects and bring them back to the starting monomer by chemical reactions we've devised that cleave the typically stable carbon-carbon bonds. By doing so, we've come closer than anyone to give the same kind of circularity to polyethylene and polypropylene that you have for polyesters in water bottles."

Hartwig, graduate student Richard J. "RJ" Conk, chemical engineer Alexis Bell, who is a UC Berkeley Professor of the Graduate School, and their colleagues will publish the details of the catalytic process in the journal Science.

A circular economy for plastics

Polyethylene and polypropylene plastics constitute about two-thirds of post-consumer plastic waste worldwide. About 80% ends up in landfills, is incinerated or simply tossed into the streets, often ending up as microplastics in streams and the ocean. The rest is recycled as low-value plastic, becoming decking materials, flowerpots and sporks.

To reduce this waste, researchers have been looking for ways to turn the plastics into something more valuable, such as the monomers that are polymerized to produce new plastics. This would create a circular polymer economy for plastics, reducing the need to make new plastics from petroleum, which generates greenhouse gases.

Two years ago, Hartwig and his UC Berkeley team came up with a process for breaking down polyethylene plastic bags into the monomer propylene—also called propene—that could then be reused to make polypropylene plastics.

This chemical process employed three different bespoke heavy metal catalysts: one to add a carbon-carbon double bond to the polyethylene polymer and the other two to break the chain at this double bond and repeatedly snip off a carbon atom and, with ethylene, make propylene (C_3H_6) molecules until the polymer disappeared. But the catalysts were dissolved in the liquid reaction and short-lived, making it hard to recover them in an active form.

In the new process, the expensive, soluble metal catalysts have been replaced by cheaper solid ones commonly used in the chemical industry for continuous flow processes that reuse the catalyst. Continuous flow processes can be scaled up to handle large volumes of material.

Conk first experimented with these catalysts after consulting with Bell, an expert on heterogeneous catalysts, in the Department of Chemical and Biomolecular Engineering.

Synthesizing a catalyst of sodium on alumina, Conk found that it efficiently broke or cracked various kinds of polyolefin polymer chains, leaving one of the two pieces with a reactive carbon-carbon double bond at the end. A second catalyst, tungsten oxide on silica, added the carbon atom at the

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end of the chain to ethylene gas, which is constantly streamed through the reaction chamber to form a propylene molecule. The latter process, called olefin metathesis, leaves behind a double bond that the catalyst can access again and again until the entire chain has been converted to propylene.

The same reaction occurs with polypropylene to form a combination of propene and a hydrocarbon called isobutylene. Isobutylene is used in the chemical industry to make polymers for products ranging from footballs to cosmetics and to make high-octane gasoline additives.

Surprisingly, the tungsten catalyst was even more effective than the sodium catalyst in breaking polypropylene chains.

"You can't get much cheaper than sodium," Hartwig said. "And tungsten is an earth-abundant metal used in the chemical industry in large scale, as opposed to our ruthenium metal catalysts that were more sensitive and more expensive. This combination of tungsten oxide on silica and sodium on alumina is like taking two different types of dirt and having them together disassemble the whole polymer chain into even higher yields of propene from ethylene and a combination of propene and isobutylene from polypropylene than we did with those more complex, expensive catalysts."

Like a string of pearls

One key advantage of the new catalysts is that they avoid the need to remove hydrogen to form a breakable carbon-carbon double bond in the polymer, which was a feature of the researchers' earlier process to deconstruct polyethylene. Such double bonds are an Achilles heel of a polymer, in the same way that the reactive carbon-oxygen bonds in polyester or PET make the plastic easier to recycle. Polyethylene and polypropylene don't have this Achilles heel—their long chains of single carbon bonds are very strong.

"Think of the polyolefin polymer like a string of pearls," Hartwig said. "The locks at the end prevent them from falling out. But if you clip the string in the middle, now you can remove one pearl at a time."

The two catalysts together turned a nearly equal mixture of polyethylene and polypropylene into propylene and isobutylene—both gases at room temperature—with an efficiency of nearly 90%. For polyethylene or polypropylene alone, the yield was even higher.

Conk added plastic additives and different types of plastics to the reaction chamber to see how the catalytic reactions were affected by contaminants. Small amounts of these impurities barely affected the conversion efficiency, but small amounts of PET and polyvinyl chloride—PVC—significantly reduced the efficiency. This may not be a problem, however, because recycling methods already separate plastics by type.

Hartwig noted that while many researchers are hoping to redesign plastics from the ground up to be easily reused, today's hard-to-recycle plastics will be a problem for decades.

"One can argue that we should do away with all polyethylene and polypropylene and use only new circular materials. But the world's not going to do that for decades and decades. Polyolefins are cheap, and they have good properties, so everybody uses them," Hartwig said. "People say if we could figure out a way to make them circular, it would be a big deal, and that's what we've done. One can begin to imagine a commercial plant that would do this."

Other co-authors of the paper are graduate students Jules Stahler, Jake Shi, Natalie Lefton and John Brunn of UC Berkeley and Ji Yang of Lawrence Berkeley National Laboratory. Shi, Hartwig and Bell are also affiliated with Berkeley Lab.

Phys Org, 29 August 2024

https://phys.org

Clever titanium gadget uses concentric rings to measure, add and multiply

2024-08-28

Less than a year ago we told you about the Tiroler, a titanium ring that's a rather clever alternative to the boring ol' tape measure. Well, its makers are back with a new take on the concept, which also performs calculations.

Known as the Mini Titanium Curve Measure Slide Rule (we'll just call it the Mini), the new device is currently the subject of a Kickstarter campaign. Both it and the Tiroler are made by Japanese company Titaner, which previously brought us a miniature adjustable spanner wrench and a little folding knife that can be opened with one hand.

The discus-shaped Mini consists of an outer ring with a smaller inner ring nested inside of it. Both rings are laser-engraved with ruler-style numeric

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markings, and can rotate independent of one another – that means you can hold the inner ring in place while rotating the outer ring around it.

Buyers are able to choose between metric and imperial versions of the device. The metric model has a circumference of 10 cm, while the larger imperial model has a circumference of five inches.

When you want to measure something, you start by aligning the 0 markings on both rings with one another. Next, you place the Mini at the beginning of the surface to be measured, holding it upright like a wheel.

You then just roll it along that surface, which can be curved or otherwise not-so-straight and/or not-so-flat. As you do so, the inner ring stays pinched between your finger and thumb, with the outer wheel doing all the rotating – it makes a satisfying snicking sound as it does so.

At the end of every full revolution of the outer ring, an integrated spring-loaded ceramic bead produces an audible, tactile click. You count those clicks in your head, as each one represents either 10 cm or five inches (depending on the model). When you get to the end of the surface being measured, you make a note of which numeric marking on the outer ring lines up with the 0 on the inner ring.

Using the metric model as an example, you then multiply the number of clicks by 10, then add the number that lines up with the inner ring's 0. So if the Mini made five clicks and ended up with 6.2 (numeral 6 and two tick marks) lined up with the 0, the measured distance would be 56.2 cm, or 562 mm.

As we mentioned earlier, the device can additionally be used to perform simple calculations. In a feat of engineering that we won't even try to understand, the two rings together form a circular slide rule that performs addition on one side of the Mini, and multiplication on the other.

It should be noted that because of its small size (which limits the room available for numeric markings) the Mini can only manage pretty basic math – stuff like 2 x 3 = 6. Most people can easily do that sort of thing in their head, so the slide rule function is more of a novelty than an actual practical tool. It's still pretty neat, though.

Buyers of the metric Mini can choose between an all-titanium model and one with a titanium outer ring and a copper inner ring. Buyers of the imperial Mini are stuck with all-titanium. Kickstarter pledges run from US$49 for the metric ti/copper model (planned retail $98) up to $65 for

the imperial ti (retail $130). If everything works out, they should ship in November.

New Atlas, 28 August 2024

https://newatlas.com

Spectroscopy study reveals electrons in cocatalyst periphery drive photocatalytic hydrogen evolution

2024-08-29

Synchronizing periodic excitations of photocatalysts with a Michelson interferometer on operando FT–IR spectroscopy, researchers led by Toshiki Sugimoto succeeded in observing and identifying the reactive electron species for photocatalytic hydrogen evolution. In contrast to previous assumptions, this study demonstrates that it is not the free electrons in metal cocatalysts but the electrons trapped in the periphery of cocatalysts that directly contribute to the photocatalysis.

The findings are published in the Journal of the American Chemical Society.

Since the discovery of photoelectrochemical hydrogen evolution by Honda and Fujishima in 1972, heterogeneous photocatalysis has been intensively investigated and is still a hot topic in science and technology. In particular, understanding of reactive electron species and active reaction sites on photocatalytic reduction reaction are vital for designing and manufacturing innovative catalysts with improved evolution activity of hydrogen as a sustainable energy carrier.

However, despite its fundamental importance, microscopic understanding of photocatalysis remains a highly challenging issue owing to an inherent difficulty in experimentally observing and extracting weak spectroscopic signals originating from the photoexcited reactive electron species.

This is predominantly due to the inevitable temperature increment for catalyst samples under actual photocatalytic reaction conditions upon continuous photon irradiation. In this case, the weak signals derived from reactive photoexcited electron species are readily overwhelmed by intense background signals originating from thermally excited nonreactive electrons.

Researchers (Dr. Hiromasa Sato and Prof. Toshiki Sugimoto) at the Institute for Molecular Science, The Graduate University for Advanced Studies, SOKENDAI succeeded in significantly suppressing the signals derived from

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thermally excited electrons and observing the reactive photogenerated electrons contributing to the photocatalytic hydrogen evolution.

This innovation was achieved by a new method based on synchronization of the millisecond periodic excitations of photocatalysts with a Michelson interferometer used for FT–IR spectroscopy. This demonstration was achieved with metal-loaded oxide photocatalysts under steam methane reforming and water splitting conditions.

Although it has long been conventionally believed that loaded metal cocatalysts function as sinks for reactive photogenerated electrons and active sites for reduction reactions, they found that the free electron species in the metal cocatalysts were not directly involved in the photocatalytic reduction reaction. Alternatively, the electrons shallowly trapped in the in-gap states of oxides contributed to enhancing the hydrogen evolution rate upon the loading of metal cocatalysts.

The electron abundance in the in-gap states, especially metal-induced semiconductor surface states, was clearly correlated to the reaction activity, suggesting that such metal-induced semiconductor surface states formed in the periphery of the metal cocatalyst play key roles in the photocatalytic hydrogen evolution.

These microscopic insights shift a paradigm on the traditionally believed role of metal cocatalysts in photocatalysis and provide a fundamental basis for rational design of the metal/oxide complex interfaces as promising platforms for nonthermal hydrogen evolution.

Furthermore, the new approach of operando infrared spectroscopy is widely applicable to other catalytic reaction systems and materials driven by the aid of photons and/or external electric field/potential. Therefore, the new approach could have great potential to uncover hidden key factors to enhance catalyst performance.

Phys Org, 29 August 2024

https://phys.org

Scientists Discover Potential Diabetes Treatment in Venom of One of the World's Deadliest Creatures

2024-08-26

Cone snail venom contains consomatin, a toxin that could lead to better, longer-lasting drugs for diabetes and hormone-related diseases by mimicking somatostatin.

A new study published in Nature Communications reveals the toxin from one of the most venomous animals on the planet may hold the key to improving drugs for diabetes and hormone disorders.

An international team of scientists led by the University of Utah identified a component within the venom of a deadly marine cone snail, the geography cone, that mimics a human hormone called somatostatin, which regulates the levels of blood sugar and various hormones in the body. The hormone-like toxin's specific, long-lasting effects, which help the snail hunt its prey, could also help scientists design better drugs for hormone disorders and diabetes.

Blueprint for Better Drugs

The somatostatin-like toxin the researchers identified could provide invaluable insights into new medications for diabetes and hormone disorders.

Somatostatin acts like a brake pedal for many processes in the human body, preventing blood sugar, various hormones, and many other important molecules from rising to dangerously high levels. The researchers found the cone snail toxin, called consomatin, works similarly, —but consomatin is more stable and specific than the human hormone, which makes it a promising blueprint for drug design.

By measuring how consomatin interacts with somatostatin's targets in human cells in a dish, the researchers found that consomatin interacts with one of the same proteins that somatostatin does. But while somatostatin directly interacts with several proteins, consomatin only interacts with one. This fine-tuned targeting means that the cone snail toxin affects hormone levels and blood sugar levels but not the levels of many other molecules.

In fact, the cone snail toxin is more precisely targeted than the most specific synthetic drugs designed to regulate hormone levels, such as drugs that regulate growth hormone. Such drugs are an important therapy for people whose bodies overproduce growth hormones. Consomatin's effects on blood sugar could make it dangerous to use as a therapeutic, but by studying its structure, researchers could start to design drugs for endocrine disorders that have fewer side effects.

Consomatin is more specific than top-of-the-line synthetic drugs—and it also lasts far longer in the body than the human hormone, thanks to the inclusion of an unusual amino acid that makes it difficult to break down.

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This is a useful feature for pharmaceutical researchers looking for ways to make drugs that will have long-lasting benefits.

Learning from Cone Snails

Finding better drugs by studying deadly venoms may seem unintuitive, but Helena Safavi, PhD, associate professor of biochemistry in the Spencer Fox Eccles School of Medicine (SFESOM) at the University of Utah and the senior author on the study, explains that the toxins' lethality is often aided by pinpoint targeting of specific molecules in the victim's body. That same precision can be extraordinarily useful when treating disease.

"Venomous animals have, through evolution, fine-tuned venom components to hit a particular target in the prey and disrupt it," Safavi says. "If you take one individual component out of the venom mixture and look at how it disrupts normal physiology, that Consomatin shares an evolutionary lineage with somatostatin, but over millions of years of evolution, the cone snail turned its own hormone into a weapon.

For the cone snail's fishy prey, consomatin's deadly effects hinge on its ability to prevent blood sugar levels from rising. And importantly, consomatin doesn't work alone. Safavi's team had previously found that cone snail venom includes another toxin that resembles insulin, lowering the level of blood sugar so quickly that the cone snail's prey becomes nonresponsive. Then, consomatin keeps blood sugar levels from recovering.pathway is often really relevant in disease." For medicinal chemists, "it's a bit of a shortcut."

Evolutionary Insights from Cone Snails

"We think the cone snail developed this highly selective toxin to work together with the insulin-like toxin to bring down blood glucose to a really low level," says Ho Yan Yeung, PhD, a postdoctoral researcher in biochemistry in SFESOM and the first author on the study.

The fact that multiple parts of the cone snail's venom target blood sugar regulation hints that the venom could include many other molecules that do similar things. "It means that there might not only be insulin and somatostatin-like toxins in the venom," Yeung says. "There could potentially be other toxins that have glucose-regulating properties too." Such toxins could be used to design better diabetes medications.

It may seem surprising that a snail is able to outperform the best human chemists at drug design, but Safavi says that the cone snails have evolutionary time on their side. "We've been trying to do medicinal

chemistry and drug development for a few hundred years, sometimes badly," she says. "Cone snails have had a lot of time to do it really well."

Or, as Yeung puts it, "Cone snails are just really good chemists."

Sci Tech Daily, 26 August 2024

https://scitechdaily.com

Thermochromic material could make indoor temperature control more energy-efficient

2024-08-28

Rice University researchers have developed a smart material that adjusts its transparency with changes in temperature, outperforming similar materials in terms of durability, transparency and responsiveness. The new polymer blend could significantly enhance energy efficiency for indoor space cooling, according to a new study published in Joule.

Cooling off can be a matter of life or death, but air conditioning -- when and if available -- already accounts for 7% of the world's energy use and 3% of carbon emissions. With temperatures hitting record highs and heat waves growing more frequent worldwide, the need for more efficient ways to keep indoor temperatures in check has also grown more urgent.

One way to mitigate the issue involves coating windows with materials that keep heat out while still allowing light to pass through. One such class of materials is thermochromics, yet existing varieties are still too expensive and short-lived to make a feasible choice for use in buildings, vehicles and wherever else needed.

The new salted polymer blend system developed by Rice engineers in the Nanomaterials Laboratory led by Pulickel Ajayan overcomes these challenges, potentially enabling the large-scale deployment of thermochromics as an energy-efficient indoor space cooling technology.

"Imagine a window that becomes less transparent as the day gets warmer, keeping interiors cool without consuming energy," said Sreehari Saju, a materials science and nanoengineering doctoral student at Rice who is a co-lead author on the study. "Our formulation leverages both organic and inorganic components to overcome the limitations of existing thermochromic materials such as short lifespans and high costs.

"Moreover, this material's thermic response is well-matched to real-world environmental demands. We think that smart windows made from this

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material could significantly reduce energy consumption in buildings, making a tangible impact on both energy costs and carbon footprint."

The researchers combined experimental methods with computational simulations to understand the material's behavior under different environmental and architectural settings. For instance, they assessed how the material would perform in specific urban areas around the world to get a sense of its potential impact when deployed at scale.

"Our approach was unique because it required a precise balance of materials and techniques that had not been previously explored in this combination, offering a new pathway for developing smart materials," said Anand Puthirath, a research scientist in the Ajayan research group and co-lead author on the study. "We conducted comprehensive experiments to characterize the properties of the material, as well environmental stability and durability testing, showing that our blend can outperform existing thermochromics."

The researchers synthesized the material by mixing two polymers with a type of salt and worked on optimizing the composition to achieve smooth transitions between transparent and opaque states with temperature fluctuations. Their findings show that the new thermochromic blend is not only highly effective in regulating solar radiation but also remarkably durable with an estimated lifespan of 60 years.

"These research findings set new benchmarks in thermochromics' durability and performance and particularly in a simple practically viable system," said Ajayan, the corresponding author on the study and Rice's Benjamin M. and Mary Greenwood Anderson Professor of Engineering and professor and department chair of materials science and nanoengineering. "Our work addresses a critical challenge in sustainable architecture, offering a practical and scalable solution for enhancing energy efficiency in buildings."

The thermochromic behavior of the material was studied in collaboration with Professor Yi Long and her doctoral student, Shancheng Wang, from the Department of Electronic Engineering at the Chinese University of Hong Kong, Sha Tin.

Science Daily, 28 August 2024

https://sciencedaily.com

Breaking open the AI black box, team finds key chemistry for solar energy and beyond

2024-08-28

Artificial intelligence is a powerful tool for researchers, but with a significant limitation: the inability to explain how it came to its decisions, a problem known as the "AI black box."

By combining AI with automated chemical synthesis and experimental validation, an interdisciplinary team of researchers at the University of Illinois Urbana-Champaign has opened up the black box to find the chemical principles that AI relied on to improve molecules for harvesting solar energy.

The result produced light-harvesting molecules four times more stable than the starting point, as well as crucial new insights into what makes them stable—a chemical question that has stymied materials development.

The interdisciplinary team of researchers was co-led by U. of I. chemistry professor Martin Burke, chemical and biomolecular engineering professor Ying Diao, chemistry professor Nicholas Jackson and materials science and engineering professor Charles Schroeder, in collaboration along with University of Toronto chemistry professor Alán Aspuru-Guzik. They published their results in the journal Nature.

"New AI tools have incredible power. But if you try to open the hood and understand what they're doing, you're usually left with nothing of use," Jackson said.

"For chemistry, this can be very frustrating. AI can help us optimize a molecule, but it can't tell us why that's the optimum—what are the important properties, structures and functions? Through our process, we identified what gives these molecules greater photostability. We turned the AI black box into a transparent glass globe."

The researchers were motivated by the question of how to improve organic solar cells, which are based on thin, flexible materials, as opposed to the rigid, heavy, silicon-based panels that now dot rooftops and fields.

"What has been hindering commercialization of organic photovoltaics is problems with stability. High-performance materials degrade when exposed to light, which is not what you want in a solar cell," said Diao. "They can be made and installed in ways not possible with silicon and can

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convert heat and infrared light to energy as well, but the stability has been a problem since the 1980s."

The Illinois method, called "closed-loop transfer," begins with an AI-guided optimization protocol called closed-loop experimentation. The researchers asked the AI to optimize the photostability of light-harvesting molecules, Schroeder said.

The AI algorithm provided suggestions about what kinds of chemicals to synthesize and explore in multiple rounds of closed-loop synthesis and experimental characterization. After each round, the new data were incorporated back into the model, which then provided improved suggestions, with each round moving closer to the desired outcome.

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"The modular chemistry approach beautifully complements the closed-loop experiment. The AI algorithm requests new data with maximized learning potential, and the automated molecule synthesis platform can generate the new required compounds very quickly. Those compounds are then tested, the data goes back into the model, and the model gets smarter—again and again," said Burke, who also is a professor in the Carle Illinois College of Medicine.

"Until now, we've been largely focused on structure. Our automated modular synthesis now has graduated to the realm of exploring function."

Instead of simply ending the query with the final products singled out by the AI, as in a typical AI-led campaign, the closed-loop transfer process further sought to uncover the hidden rules that made the new molecules more stable.

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"We're using AI to generate hypotheses that we can validate to then spark new human-driven campaigns of discovery," Jackson said.

"Now that we have some physical descriptors of what makes molecules photostable, that makes the screening process for new chemical candidates dramatically simpler than blindly searching around chemical space."

To test their hypothesis about photostability, the researchers investigated three structurally different light-harvesting molecules with the chemical property they identified—a particular high-energy region—and confirmed that choosing the proper solvents made the molecules up to four times more light-stable.

"This is a proof of principle for what can be done. We're confident we can address other material systems, and the possibilities are only limited by our imagination. Eventually, we envision an interface where researchers can input a chemical function they want and the AI will generate hypotheses to test," Schroeder said.

"This work could only happen with a multidisciplinary team, and the people, resources and facilities we have at Illinois, and our collaborator in Toronto. Five groups came together to generate new scientific insight that would not have been possible with any one of the sub-teams working in isolation."

Phys Org, 28 August 2024

https://phys.org

Investigating the molecular basis of a nice cup of tea

2024-08-25

As a keen tea drinker I was intrigued by a January 2020 tweet in which @ andrechemist wondered if a tetrahedral teabag produced a better cup of tea. The question sent me into the literature to see what chemists knew about the shape of teabags and the resulting brew. In fact, just what did chemists know about making tea more generally?

Quite a lot as it turns out. This should not have surprised me as tea is the most popular beverage in the world after water (a statistic nearly every paper on tea I read cited). In the end I wrote my own version of George Orwell's 1946 essay, 'A Nice Cup of Tea' for Nature Chemistry. That essay grew into my book Steeped: The chemistry of tea.

There is a vast chemical literature on tea: I read some 500 papers. To flesh out what I was reading, I did some experiments of my own. I measured cooling curves for teapots of different materials, spiked my tea with extra

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doses of its naturally occurring amino acid l-theanine to see if it affected the flavour (researchers disagreed, but I could taste the difference) and sampled heavy water to determine if it is sweet (it is). Given its price tag I drew the line at buying deuterium-depleted water to see if that produced an exceptional cup of tea as one author suggested, and a lack of snow the past two winters kept me from scraping it off plum blossoms to reproduce a famously extraordinary cup detailed in an 8th century Chinese manuscript.

The biggest challenge I faced in writing Steeped – beyond the daunting scope of the literature – was how to present the chemistry in such a way that someone who had not taken a chemistry course could appreciate what was happening in a cup of tea on the molecular level. I settled on highlighting four big ideas that chemists use to explain the behaviour of molecules: atoms make up everything, opposites attract, getting close matters, and molecular function depends on molecular structure. I wrote an introductory chapter that fleshes out these concepts and provides a short course in how to read chemical structures. In case people were daunted by even that much chemistry, I wrote a three paragraph TL;DR that was just enough (I hoped) to get them through. I wanted not only to help non-chemists navigate the chemistry in the book, but to let them catch a glimpse of the world as chemists see it. I hope that readers without a science background will be able to wield these concepts to understand other everyday chemistry.

Researching Steeped changed my own tea making habits. My experiments measuring the cooling curves drove home to me the importance of pre-warming the teapot or the cup whenever possible. If I don't, the temperature in my favorite Japanese cast-iron tetsukyūsu quickly drops below the optimum temperature for extracting caffeine and other desirable compounds. These days I reach more often for a double-walled glass pot that not only keeps the tea hot while it brews, but also keeps it at a drinkable temperature longer without the need for a tea cozy.

I have also become a more agitated brewer of tea. I repeatedly dunk teabags and swish my tea basket infuser as the tea steeps in order to expose the tea leaves more evenly to the solvent and extract more catechins—tea's signature antioxidants. Finally I unscrew the lid on my travel mug when I can to inhale the volatile calming compounds such as linalool found in the steam.

While writing Steeped certainly enhanced my enjoyment of a cup of tea, there were several disquieting discoveries along the way. There are

the remains of lots of bugs in my tea – the DNA of hundreds of different insects have been identified in tea leaves. I also now know how closely the white film that appears on tea when water is heated in the microwave resembles bathtub scum. Though that also means that the remedy is the same for both, some citric acid to chelate those hard water ions.

I particularly enjoyed encountering other women connected to the chemistry of tea. The earliest paper I read was from 1885, a careful analysis of an infusion of tea by Wilhelmina Green, a chemist I wish I knew more about. And while the invention of the modern teabag is usually credited to Thomas Sullivan in 1908, a US patent for such a teabag was issued to Roberta Lawson and Mary McLaren five years earlier.

And to answer the question that kicked off this project, it is not so much the shape of the teabag that matters as the size. To use one of the big ideas of chemistry, the tea leaves need enough space to get close to the water. Agitate well and enjoy a better cup of tea.

Chemistry World, 25 January 2024

https://chemistryworld.com

Old books can have unsafe levels of chromium, but readers' risk is low

2024-08-18

Old books can be beautiful to look at. But handle with care — they just might be toxic.

The covers of Victorian-era books are already known to sometimes have pigments that contain toxic heavy metals such as lead, chromium and arsenic. But when researchers recently assessed a collection at their university's main library, they found toxic metal concentrations on some tomes that exceeded safe levels.

"I think it's very important for librarians to be aware of those risks," says Leila Ais, an undergraduate student studying biochemistry at Lipscomb University in Nashville who presented the team's findings August 18 at the American Chemical Society meeting in Denver.

Librarians approached the team about testing old, brightly colored books in the university's collection. The researchers used a handheld machine called an X-ray fluorescence spectrometer to detect metals in the covers of 26 books. Additional laboratory studies helped the team determine the amount of each metal compound present in the cover.

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In the golden-yellow covers of some books, Ais and colleagues found crocoite — a compound containing the toxic metals lead and chromium — and lead sulfate, two compounds that make up a pigment called chrome yellow. Post-Impressionist painter Vincent van Gogh notably used chrome yellow pigments in his sunflowers series (SN: 3/23/16).

"[One] thing that surprised me is how concentrated [the metals in] some of the books are," Ais says. In the most metal-rich book cover, the chromium concentration was around 50 parts per million, well above the 4–25 ppm that can cause skin reactions, according to the U.S. Centers for Disease Control and Prevention.

But that doesn't necessarily mean library patrons are in danger. Chrome yellow doesn't flake off the covers easily, so the risk of inhaling particles or transferring those heavy metals to your hands is low, says Rosie Grayburn, an analytical materials scientist at Winterthur Museum in Delaware and with the Poison Book Project, a research initiative at Winterthur and the University of Delaware to identify toxic pigments in book covers. Other pigments, such as arsenic-based emerald green, flake more easily and carry a greater risk for exposure, she says.

Lipscomb's team plans to contribute its findings to the Poison Book Project after running a few more tests. In the meantime, library staff have sealed books that might contain harmful compounds in plastic bags and removed ones known to contain toxins from circulation.

Science News, 18 August 2024

https://sciencenews.org

Biomass-Based Material Captures CO2 Without Extreme Pressures or Temperatures

2024-08-27

A new, biomass-based material developed by FAMU-FSU College of Engineering researchers can be used to repeatedly capture and release carbon dioxide.

The material is primarily made from lignin, an organic molecule that is a main component of wood and other plants, and it can take up carbon dioxide (CO2) from concentrated sources or directly from the air. The research was published by Advanced Materials.

"The beauty of this work is the ability to precisely control the capture and release of CO2 without high pressure or extreme temperatures," said study co-author Hoyong Chung, an associate professor in the FAMU-FSU College of Engineering. "Our testing showed that this material's structure stayed the same even after being used multiple times, making this a promising tool for mitigating carbon emissions."

In previous research, Chung's team developed a lignin and CO2-based polymer that represented a potential alternative to traditional petroleum-based plastic.

This paper takes that research further, showing the possibility of reversing the process and of reusing the material to absorb CO2 again in the future.

Because it is found in plants, lignin is abundant and cheap, and it is often harvested as a byproduct from wood processing. Scientists are working to find new ways to use this natural resource.

One gram of the material developed by Chung's team captured 47 milligrams — about 5% of the weight of the original material — of CO2 from a concentrated source and 26 milligrams from exposure to ambient air. The absorbed CO2 can be permanently sequestered, or it can be released for use in various applications, such as manufacturing, agriculture and others.

Researchers were surprised by the release mechanism. While using nuclear magnetic resonance spectroscopy to analyze a sample, they saw bubbles appear when the sample was heated.

"That sparked our curiosity," Chung said. "What's going on here? Why do we see these little bubbles every time we try to analyze this polymer?"

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Further investigation revealed that heat was causing the material to release CO2. The researchers investigated the reaction and found that by controlling the heat applied to the sample, they were able to control the amount of CO2 released. They also showed the possibility of using that captured gas in other reactions.

It only takes temperatures of about 60 degrees Celsius at normal atmospheric pressure to release the CO2, meaning high temperatures and pressures aren't necessary for the reuse process. This CO2 release temperature can be increased or decreased for different applications.

"This is like a sponge for CO2, absorbing it, releasing it and drying up so it can capture more," Chung said. "It's fascinating to see what is possible with this material."

Reference: Ghorai A, Chung H. Ionic lignin polymers for controlled co 2 capture, release, and conversion into high-value chemicals. Adv Mater. 2024:2406610. doi: 10.1002/adma.202406610

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Technology Networks, 27 August 2024

https://technologynetworks.com

Prozac pollution is disrupting fish reproduction

2024-08-27

The law of unintended consequences gained new appreciation today when a five-year international study was published in the Journal of Animal Ecology detailing how long-term exposure to pharmaceutical pollutants can have dramatic consequences for marine wildlife.

It seems that waterway pollution resulting from the widely prescribed antidepressant fluoxetine (Prozac) is having catastrophic effects on fish behavior and fish reproduction, with Guppy males growing a larger sex organ (the gonopodium – a fin-like organ used to fertilize the female), reducing the velocity of their sperm and their overall body condition, and inhibiting their behavioral plasticity (their ability to adapt).

The general body condition of male Guppies is critically important for mating and for fighting with other males, threatening their overall survival.

The study's co-lead author, Dr Upama Aich from the Monash University School of Biological Sciences in Australia, said chemicals were "being dumped into our waterways every day" and the changes observed in guppies at low concentrations of fluoxetine should be taken as a warning about their ability "to live and survive and thrive in a polluted environment."

Pharmaceutical pollutants have become a pervasive issue in rivers, lakes and oceans worldwide but until this study, the impact of these chemicals on aquatic wildlife, particularly on behavior and reproductive success, has not been clear.

"Fluoxetine exposure also significantly reduced the behavioral plasticity of guppies, leading to a lower capacity of the individuals to adjust their own activity and risk-taking behaviors across contexts," said the paper's co-author, Assistant Professor Giovanni Polverino from the University of Tuscia.

The findings highlight the need for a more comprehensive approach to evaluating the ecological and evolutionary consequences of pharmaceutical pollution. As human activities continue to introduce new pollutants into the environment, understanding their effects on wildlife is crucial for preserving biodiversity and ensuring the health of ecosystems.

New Atlas, 27 August 2024

https://newatlas.com

A way to recover silver from dead solar panels with 98% efficiency

2024-08-28

A multi-institutional team of chemists, metallurgists and engineers has developed a highly efficient way to retrieve silver from dead solar panels. Their paper is published in Environmental Technology & Innovation.

As climate change progresses, scientists seek to replace fossil fuels with renewable resources, including solar power. But the development of these technologies has led to new environmental problems, such as what to do with solar panels after their useful life expires.

Prior research has shown that some solar panel components are relatively easy to recycle, including the iron, steel and aluminum used to make brackets, racks and other support systems.

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Unfortunately, other components are more challenging to recover, such as the silver used in electrical circuits—it must be separated from the circuitry and the copper that is almost always present. Thus, these materials are seldom recycled. In this new study, a team in Italy developed a relatively inexpensive way to recover the silver used in solar panels.

The process involves the use of a base-activated persulfate along with ammonia. In this way, the persulfate could serve as the oxidizing agent. As a reaction proceeds, copper oxide is produced, which serves as a protective layer, preventing leaching of the copper.

To find the right amounts of each of the materials to use in the process, the researchers conducted multiple reactions using different variables, such as ammonia concentrations, while keeping other variables such as stirring speed and temperature even.

After much experimentation, the team found the right combination of factors—ammonia at a concentration of 0.5 M and potassium persulfate at 0.2 mol per liter, and a reaction time of one hour. Under these conditions, the reaction results in the separation of 85% of the silver in a sample.

The team then carried out an electrodeposition-redox replacement to increase the percentage to 98.7%. Via scanning electron microscope, the team confirmed the enrichment of the silver particles.

Phys Org, 28 August 2024

https://phys.org

Engineers develop all-in-one solution to catch and destroy 'forever chemicals'

2024-08-28

Chemical engineers at the University of British Columbia have developed a new treatment that traps and treats PFAS substances -- widely known as "forever chemicals" -- in a single, integrated system.

Per- and polyfluoroalkyl substances (PFAS) are widely used in manufacturing consumer goods like waterproof clothing due to their resistance to heat, water and stains. However, they are also pollutants, often ending up in surface and groundwater worldwide, where they have been linked to cancer, liver damage and other health issues.

"PFAS are notoriously difficult to break down, whether they're in the environment or in the human body," explained lead researcher Dr. Johan

Foster, an associate professor of chemical and biological engineering in the faculty of applied science. "Our system will make it possible to remove and destroy these substances in the water supply before they can harm our health."

Catch and destroy

The UBC system combines an activated carbon filter with a special, patented catalyst that traps harmful chemicals and breaks them down into harmless components on the filter material. Scientists refer to this trapping of chemical components as adsorption.

"The whole process is fairly quick, depending on how much water you're treating," said Dr. Foster. "We can put huge volumes of water through this catalyst, and it will adsorb the PFAS and destroy it in a quick two-step process. Many existing solutions can only adsorb while others are designed to destroy the chemicals. Our catalyst system can do both, making it a long-term solution to the PFAS problem instead of just kicking the can down the road."

No light? No problem

Like other water treatments, the UBC system requires ultraviolet light to work, but it does not need as much UV light as other methods.

During testing, the UBC catalyst consistently removed more than 85 per cent of PFOA (perfluorooctanoic acid, a type of forever chemical) even under low light conditions.

"Our catalyst is not limited by ideal conditions. Its effectiveness under varying UV light intensities ensures its applicability in diverse settings, including regions with limited sunlight exposure," said Dr. Raphaell Moreira, a professor at Universität Bremen who conducted the research while working at UBC.

For example, a northern municipality that gets little sun could still benefit from this type of PFAS solution.

"While the initial experiments focused on PFAS compounds, the catalyst's versatility suggests its potential for removing other types of persistent contaminants, offering a promising solution to the pressing issues of water pollution," explained Dr. Moreira.

From municipal water to industry cleanups

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The team believes the catalyst could be a low-cost, effective solution for municipal water systems as well as specialized industrial projects like waste stream cleanup.

They have set up a company, ReAct Materials, to explore commercial options for their technology.

"Our catalyst can eliminate up to 90 per cent of forever chemicals in water in as little as three hours -- significantly faster than comparable solutions on the market. And because it can be produced from forest or farm waste, it's more economical and sustainable compared to the more complex and costly methods currently in use," said Dr. Foster.

The research was supported by an NSERC Discovery grant and was recently published in Nature Communications Engineering.

Science Daily, 28 August 2024

https://sciencedaily.com

New device may let everyday folks check their water for microplastics

2024-08-28

While an increasing number of people are becoming concerned about microplastic pollution in their drinking water, it's one of those things that the average person can't check for themselves. That could soon change, however, if a new prototype device reaches production.

By definition, microplastics are fragments of plastic smaller than 5 millimeters in diameter.

Found in waterways around the world, they come from a number of sources. These include chunks of floating plastic waste that break down into smaller pieces; products such as toothpaste which contain plastic microbeads; synthetic clothing that sheds fibers while being washed; and car tires that release bits of rubber which make their way into storm sewers.

Researchers are still trying to understand how people's health may be affected by ingesting the particles in and of themselves. That said, harmful bacteria are often drawn to microplastics, living on or around the particles – and we definitely shouldn't be eating or drinking those microbes.

Presently, the only methods of counting the number of microplastics in water samples require expensive lab-based equipment operated by trained technicians. Dr. Tianxi Yang and colleagues at Canada's University of British Columbia (UBC) recently set out to change that.

The result is a small 3D-printed box that contains a wireless digital microscope, a green LED, and a device known as an excitation filter. Machine-learning-based software on a linked smartphone analyzes images transmitted by the microscope.\

Only a tiny amount of water is required (less than one drop), to which a solution of tannic acid, zirconium atoms and rhodamine B is added. When that mixture is exposed to green light from the LED, all of the microplastics present within it fluoresce, making them highly visible.

The smartphone software counts the number of fluorescence-showing pixels in the microscope images, thus allowing it to determine both the size and amount of particles in the sample. Within less than 20 minutes, it provides a readout that can be easily understood by scientists and laypeople alike.

In a test of the technology, the device was used to analyze distilled water that had been boiled and poured into polystyrene cups, then left to cool for 30 minutes. Based on the number of microplastics detected in the samples, it was determined that each cup released "hundreds of millions" of nano-sized particles into the 50 ml (1.7 oz) of water it contained.

While these particular tests were looking for polystyrene particles, the scientists state that the software could be tweaked to detect other plastics such as polyethylene and polypropylene. A paper on the study was recently published in the journal ACS Sensors.

And should you be wondering what a user would do if a commercial version of the device did show that their water was full of microplastics … well, last year UBC announced the development of a plant-based filter that removes almost 100% of such particles from water.

Source: UBC

New Atlas, 28 August 2024

https://newatlas.com

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Polyethylene Could Replace Bamboo For Oyster Farming Rafts

2024-08-28

Amid the rising human population and pressure on food supplies, the world can't be everyone's oyster. But perhaps there might be more oysters to eat if an Osaka Metropolitan University-led research team's findings mean sturdy plastic rafts will be used in their farming.

Conventional oyster farming uses bamboo rafts with additional flotation devices such as Styrofoam. Though relatively affordable, these rafts can be damaged in typhoons. The OMU-led researchers propose a polyethylene raft that keeps costs manageable but is about five times more durable than a bamboo raft.

OMU Graduate School of Engineering Associate Professor Yasunori Nihei led the team in running the numerical analysis and verifying the performance by building a test model of the polyethylene raft.

"The numerical analysis technique developed in this research is expected to be applicable not only to oysters, but also to the performance evaluation of aquaculture ponds," Professor Nihei proclaimed. "We hope our efforts will contribute greatly to the future growth of the aquaculture industry."

Reference: Tamura H, Iwamatsu S, Iijima K, Nihei Y. Motion characteristics and deformation performance of highly flexible polyethylene rafts for oyster farming. Ocean Eng. 2024;310:118537. doi: 10.1016/j.oceaneng.2024.118537

Technology Networks, 28 August 2024

https://technologynetworks.com

Chemists achieve PFAS-free synthesis of fluorinated pharmaceutical and agrochemical compounds

2024-08-29

Chemists at the University of Amsterdam have developed a method to furnish a range of molecules with a trifluoromethyl group attached to a sulfur, nitrogen or oxygen atom. Their procedure, which is published in Science, avoids the use of PFAS reagents. It thus provides an environmentally friendly synthesis route for pharmaceutical and

agrochemical compounds that rely on the presence of the trifluoromethyl group.

The straightforward and effective method was developed in the Flow Chemistry group at the Van 't Hoff Institute for Molecular Sciences led by Prof. Timothy Noël, in cooperation with researchers in Italy, Spain and the UK, both from academia and industry. Applying the principles of flow chemistry, where reactions take place in closed systems of small tubes, makes for safe and controlled chemistry. It also offers greater versatility and flexibility over more common procedures using traditional chemical glassware.

More environmentally friendly

Many pharmaceutical compounds (such as anti-depressants) as well as agrochemical compounds (such as pesticides) benefit from the presence of a trifluoromethyl (-CF3) group. It enhances hydrophobicity and increases metabolic stability, thus improving efficacy and lowering the required dose or concentration.

To introduce the fluorine atoms in these molecules, their synthesis often requires bespoke fluorinated reagents. Many of these are among the family of PFAS compounds and thus will face future legislation. The synthesis protocol now presented in the paper provides a viable alternative since it only requires cesium fluoride salt as the fluorine source. Such PFAS-free synthesis of fluorinated agents can provide an environmentally more friendly option for the synthesis of pharmaceutical compounds, which motivated scientists from AstraZeneca to participate in the research.

In addition, the new synthesis protocol enables coupling of the CF3 group through a sulfur (S), nitrogen (N) or oxygen (O) atom. Such fluorinated motifs confer unique features to drug molecules and agrochemicals, impacting their lipophilicity, oxidation resistance, and acid-base properties.

Integrated flow system

The paper presents a versatile microfluidic flow module for generating reactive N–, S– and O–CF3 anions. These are prepared in a packed bed flow reactor containing the cesium fluoride salt. Appropriate (S, O or N containing) precursors are then led through this reactor. They are fluorinated with high efficiency due to the high surface area of the salt in the packed bed as well and the improved mixing of the organic

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intermediates. Importantly, this approach also offers enhanced safety as all formed intermediates are contained within the microfluidic system.

Another important feature of the system is the integration of the anion generating module with a downstream reaction module. There, the N–, S– or O–CF3 anions react with appropriate substrates to achieve pharmaceutical and agrochemical active ingredients as the desired end products.

Implementation in an academic and industrial context

In combination, the anion generator module and the downstream reactor provide a streamlined platform for the derivatization of molecules bearing N–, S– and O–CF3 motifs. This innovative approach is poised to impact the development of new pharmaceutical drugs by enhancing their properties while improving safety and sustainability in their production processes.

In their paper, the researchers report the combination of various anions with a range of substrates, resulting in multiple fluorinated products with relevance to pharmaceutical and agrochemical syntheses. In many cases, the research team was able to report very satisfactory yields. Moreover, the operational parameters (e.g., reaction times) offer a good prospect for actual implementation in an academic as well as an industrial context.

Phys Org, 29 August 2024

https://phys.org

Is Coffee Healthy for You? New Research Reveals It Depends on Your Genetics

2024-08-26

When it comes to your genetics, the answer is complicated.

Coffee drinking is a heritable habit, and one that carries a certain amount of genetic baggage.

Caffeinated coffee is a psychoactive substance, notes Sandra Sanchez-Roige, Ph.D., an associate professor in the University of California San Diego School of Medicine Department of Psychiatry. She is one of an international group of researchers who compared coffee consumption characteristics from a 23andMe database with an even larger set of records in the United Kingdom. She is the corresponding author of a study recently published in the journal Neuropsychopharmacology.

Hayley H. A. Thorpe, Ph.D., is the lead author on the paper. Thorpe, of the Department of Anatomy and Cell Biology, Schulich School of Medicine and Dentistry at Western University in Ontario, explained that the team collected genetic data as well as self-reported coffee-consumption numbers to assemble a genome-wide association study (GWAS). The idea was to make connections between the genes that were known to be associated with coffee consumption and the traits or conditions related to health.

"We used this data to identify regions on the genome associated with whether somebody is more or less likely to consume coffee," Thorpe explained. "And then identify the genes and biology that could underlie coffee intake."

Genetic Influences on Coffee Drinking

Abraham Palmer, Ph.D., is also a lead researcher on the paper and a professor in the UC San Diego School of Medicine Department of Psychiatry. He said that most people are surprised that there is a genetic influence on coffee consumption. "We had good reason to suspect from earlier papers that there were genes that influence how much coffee someone consumes," he said. "And so, we weren't surprised to find that in both of the cohorts we examined there was statistical evidence that this is a heritable trait. In other words, the particular gene variants that you inherit from your parents influence how much coffee you're likely to consume."

Sanchez-Roige said the genetic influence on coffee consumption was the first of two questions the researchers wanted to address.

"The second is something that coffee lovers are really keen on learning," Sanchez-Roige said. "Is drinking coffee good or bad? Is it associated with positive health outcomes or not?"

The answer is not definitive. The group's genome-wide association study of 130,153 U.S.-based 23andMe research participants was compared with a similar UK Biobank database of 334,649 Britons, revealing consistent positive genetic associations between coffee and harmful health outcomes such as obesity and substance use. A positive genetic association is a connection between a specific gene variant (the genotype) and a specific condition (the phenotype). Conversely, a negative genetic association is an apparent protective quality discouraging the development of a condition. The findings get more complicated when it comes to psychiatric conditions.

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Challenges in Data Comparison and Cultural Differences

"Look at the genetics of anxiety, for instance, or bipolar and depression: In the 23andMe data set, they tend to be positively genetically correlated with coffee intake genetics," Thorpe said. "But then, in the UK Biobank, you see the opposite pattern, where they're negatively genetically correlated. This is not what we expected."

She said there were other instances in which the 23andMe set didn't align with the UK Biobank, but the greatest disagreement was in psychiatric conditions.

"It's common to combine similar datasets in this field to increase study power. This information paints a fairly clear picture that combining these two datasets was really not a wise idea. And we didn't end up doing that," Thorpe said. She explained that melding the databases might mask effects, leading researchers toward incorrect conclusions — or even canceling each other out.

Sanchez-Roige says the researchers have some ideas about how the differences in results arose. To begin with, there was an apples-and-oranges aspect to the surveys. For instance, the 23andMe survey asked, "How many 5-ounce (cup-sized) servings of caffeinated coffee do you consume each day?" Compare it to the UK Biobank's "How many cups of coffee do you drink each day? (Include decaffeinated coffee)"

Beyond serving size and the caffeinated/decaf divide, the surveys made no accommodations for the various ways coffee is served. "We know that in the U.K., they have generally higher preference for instant coffee, whereas ground coffee is more preferred in the U.S.," Thorpe said.

"And then there's the frappuccinos," Sanchez-Roige added, citing the American trend of taking coffee loaded with sugary additives. Palmer mentioned other caffeinated drinks, especially in the context of the UK Biobank, tea, none of which were included in the GWAS, which addressed only coffee. Palmer added that the GWAS demonstrates the relationship between genotype and phenotype is more different than the relationship between coffee and tea.

Sci Tech Daily, 26 August 20

https://scitechdaily.com

The GLP-1 weight loss revolution

2024-08-28

Glucagon-like peptide-1 agonist drugs, such as semaglutide, could save countless lives at risk due to diabetes and obesity. Rachel Brazil looks at the difficulties in making the peptides themselves, and what's coming next

It's rare that the public becomes aware of a recently approved drug, but the chances are you've heard of semaglutide, or its tradename Ozempic, one of a growing number of drugs that replicates the action of the natural hormone, glucagon-like peptide-1. They've been widely covered in the global media as a much sought-after solution to losing weight. For some this is a matter of vanity, but for the estimated one billion people suffering from obesity in the world, it could prevent serious ill-heath and death.

GLP-1 is released in the gut in the presence of glucose and stimulates the release of insulin from pancreatic B cells, enabling fine control of blood sugar levels. The first drug targeting the GLP-1 receptor was exenatide, released in 2005 as a twice-daily injection to treat type II diabetes. It was discovered in the saliva of the Gila monster, a venomous lizard found in the American southwest, although no one knows why the lizard produces a molecule that replicates the action of GLP-1 when injected twice a day. For at least 20 years, pharma companies led by Novo Nordisk and Eli Lilly have been trying to find a better alternative. Novo was first to hit the jack pot with semaglutide, approved to treat diabetes in the UK in 2019 (as Ozempic).

The attention it is now receiving stems from its ability to promote weight loss more effectively than any previous drug therapy. In a clinical trial participants lost an average of 15% of their body weight after 68 weeks. Now production cannot keep up with demand for this instant blockbuster peptide drug, also marketed for weightloss as Wegovy, and the similar GLP-1 drug developed by Lilly, tirzepatide (Zepbound or Mounjaro). For pharma, the race is now on to ramp up and optimise production while developing the next generation of these drugs.

Early promise

The GLP-1 hormone is part of the intricate mechanism in our bodies to distribute glucose, but avoid the toxicity associated with high concentrations in the bloodstream. The 30-residue peptide regulates the release of insulin, but doesn't stick around. 'Its effects are so powerful that there are mechanisms that very quickly disable it,' explains chemist Sam Gellman from the University of Wisconsin–Madisonin the US. The enzyme

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dipeptidyl peptidase 4 (DPP-IV) cleaves it between the second and third residues which renders it inactive within several minutes, and explains why GLP-1 cannot be used as a drug itself.

Efforts to synthesise a more chemically stable analogue resulted in the drug liraglutide, a daily injection for diabetics released by Novo Nordisk in 2015. Attaching a 16-carbon side chain (palmitic acid) to the peptide allowed the molecule to bind to the abundant blood protein albumin and keep it in circulation. By 2004, Novo had selected its new lead candidate from 217 peptides, which became the once weekly injection semaglutide. This variant incorporates an 18-carbon hydrophobic fatty acid side chain (1,18-octadecanedioic acid) to bind the peptide to albumin, which is akin to 'attaching a house to GLP-1', says chemist Krishna Kumar from Tufts University in Massachusetts, US.

The other crucial modification that increases its stability is substituting the eighth residue, an alanine, with amino-isobutyric acid (AIB) which has an additional methyl group making the alpha carbon quaternary. 'Just that one small subtle substitution, enhancing the molecular weight by 14 daltons, substantially increased the stability of the the peptide,' says Paul Levine, a chemist at peptide company Insamo in California, US. The change prevents DPP-IV cleaving the molecule, resulting in a previously unheard of half-life of a week. Novo has even been able to produce an oral formulation.

'People report they're just not that interested in food since they started taking drugs like semaglutide,' says Stefan Trapp, a neuroscientist at University College London in the UK. He is trying to develop a greater understanding of this process and particularly the role of the brain. These drugs may have even broader therapeutic uses. A recent study shows people with obesity taking GLP-1 drugs are 20% less likely to suffer a cardiovascular event, and studies are under way for their use to treat the liver disease non-alcoholic steatohepatitis, as well as the neurodegenerative conditions Parkinson's and Alzheimer's. Plus there are indications it could even treat addiction.

Production problems

Anyone trying to get hold of these drugs will be aware of the recent shortages. There is huge demand, but producing peptide drugs in large quantities is proving a challenge for Novo and Lilly. Kumar says Novo insiders have told him the demand is about 20 times higher than the current supply. Semaglutide is made by recombinant expression of most of the peptide sequence in yeast, followed by several chemical

modifications. The amino acid sequence is amended to switch a lysine for an arginine, leaving only one lysine in the sequence, which is used to introduce the fatty acid side chain. Then the first two amino acids including the AIB unit are also added.

For tirzepatide, approved in the UK in March, Lilly has opted for a chemical synthesis. The molecule consists of 39 amino acids, with the non-natural AIB incorporated at positions 2 and 13, which make it difficult to make using cheaper recombinant technologies. But the alternative chemical synthesis is not easy at scale. The solid phase peptide synthesis (SPPS) method attaches the first amino acid to a resin bead, with stepwise reactions to lengthen the chain. To prevent polymerisation of each added amino acid, its alpha amino group and reactive side chains are masked with a temporary protecting group. Between each stage the resin is filtered and washed to remove byproducts, excess reagents and the terminal protecting groups, and the cycle is repeated until the final peptide is cleaved from the resin and purified using chromatography.

With so many steps the process has a failure rate of about 20% for peptides above 30 amino acids, leaving a lot of impurities to remove. Purifying long peptides is difficult, plus these GLP-1 peptide drugs have been modified to include a fatty acid side chain, and 'lipids themselves can be very difficult to purify, because they're very hydrophobic, and tend to stick to the [purification] column,' says Levine.

Lilly has gone for a hybrid method, outsourcing the manufacture of several peptide fragments and then assembling the fragments using liquid-phase peptide synthesis (LPPS). Instead of being bound to resin, the non-side-chain carboxyl functionality of the amino acid in the peptide fragment is protected as a bulky ester. Once reacted, a ceramic membrane is used as a nanofilter to separate based on molecular weight and hydrophobicity, removing smaller impurities and allowing further peptides to be coupled in the liquid phase. In a recent publication Lilly says the hybrid SPPS/LPPS method allows for high purities with a yield greater than 70%.

Both companies are increasing peptide production capacity. Novo Nordisk is spending $6 billion (£4.7 billion) on a new 170,000m2 facility at its Kalundborg site in Denmark to be completed in 2029. Along with other investments, Novo says it will 'future-proof' the company's supply. Lilly recently completed a new hybrid peptide manufacturing facility at its existing site at Kinsale in Ireland, together with expansion in the US and Germany.

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One important issue is how to make peptides in a greener way as well as at lower cost. SPPS uses large quantities of organic solvents – often five washes per step, which drives up the waste and environmental footprint for making peptides. Lilly has been investing in new technologies to improve the LPPS method by optimising the separation of the growing peptide chain. One method, known as molecular hiving, tags the first amino acid with long soluble hydrophobic anchor molecules, which can later be removed. The growing tagged peptides can be precipitated in aqueous solution and other impurities rinsed away before the next cycle starts. Overall the process uses fewer reagents and solvents.

The race to generics and alternatives

Novo Nordisk's first GLP-1 drug liraglutide will be off patent in November and in June Teva Pharmaceuticals received US authorisation to market the first-ever generic version, to treat diabetes. Other companies are following suit. Pharmaceutical chemist Walter Cabri from the University of Bologna in Italy says many generics companies are working on full chemical syntheses of liraglutide. The other big prize will be semaglutide, which goes off-patent in Europe in 2031.

Cabri is a consultant for the intravenous generic drug company Fresenius Kabi, and is working with it on novel peptide production methods. He says companies need to find methods that give them freedom to operate – that are not under patent to other companies. 'We are working on the hybrid synthesis, where we make some [peptide] pieces with SPPS and then we will couple [them] together with an enzyme.' So far they have done this for liraglutide using a unique ligation point – the site where the enzyme couples two natural amino acids.

Others are looking at alternative ways to stabilise GLP-1 drugs that might prove easier to produce. Akhter Hossain at the University of Melbourne in Australia has suggested rather than adding a fatty acid side chain, a glycan group may work instead – which is more hydrophilic and therefore easier to dissolve and purify. 'In vivo, it is not actually going to bind to albumin, but [the glycan] has sialic acid moieties, which also reduces the liver metabolism, and thus increases the circulating half-life in the blood,' explains Melbourne researcher Chaitra Chandrashekar, who carried out the work.

They were able to do the synthesis by joining just two peptide fragments with an enzyme, omniligase-1, which catalyses amide bond formation, using fewer steps than most other methods. Chandrashekar found the increase in yield was 10-fold. 'We did use the same protocol to also make

semaglutide; however, we could isolate only 4% of it, while we could isolate almost 45% of our glyco GLP-1.' Rat studies show blood glucose lowering effects similar to semaglutide, although the half-life is not yet established. If it does compare favourably this might provide the kind of production boost that is going to be needed.

Multiple targets

The next generation of GLP-1 drugs is already entering the clinic – with a shift to dual and triple agonists. Drugs able to activate a number of receptors seem to perform better. Already authorised, Lilly's tirzepatide targets both GLP-1 and the glucose-dependent insulinotropic polypeptide (GIP) receptor, which has a complementary role in stimulating insulin secretion and reducing appetite.

Lilly is following this with retatrutide, a triple agonist, which has completed phase 2 trials for treating obesity and cardiovascular disease. It additionally targets the glucagon (GCG) receptor, another part of the machinery to control blood glucose levels in line with energy expenditure. A recent trial comparing tirzepatide to semaglutide showed a greater increase in weight loss after a year, with losses of 15.3% with tirzepatide compared with 8.3% for semaglutide. Lilly's phase 2 retatrutide trial achieved up to 17.5% mean weight reduction at 24 weeks.

Using one molecule to target all these receptors seems to work because their structures are all based on similar long alpha helices. 'If you squint and look at these receptors, they all look essentially identical, with small changes,' says Kumar. The strategy is then to mix and match amino acid residues from the three natural peptides, 'I call this a Frankenstein strategy, you're taking the pieces from here, pieces from there,' says Gellman.

Modifications are also being designed to create biased agonists. 'When you activate the receptor, a lot of proteins bind to it intracellularly, but if you bind and only recruit the protein that you want, it can go through a more selective pathway,' explains Levine. This is one strategy for reducing the nausea side effects which are commonly experienced with GLP-1 drugs. With the GLP-1 receptor there is the pathway linked to insulin control, but also a pathway that recruits the signalling molecule beta arrestin, which causes the side effects but also results in the whole receptor and drug molecule being taken inside the cell, shutting down any further activity. The challenge is to bias the receptor response and so reduce these competing signalling mechanisms.

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Kumar has found he can design bias into GLP-1 analogues by simply alkylating or trifluoroalkylating the N-terminal amino acid using an alkyl halide. He has created a library of DPP-IV resistant peptides that bind at the receptor sites. 'We have unimolecular, dual agonist, tri-agonist, [and] tetra-agonists, where you can just add an alkyl group, and then you can tune GLP-1 receptor [sensitivity] up or down,' says Kumar. You can do the same thing with GIP, GCG and peptide tyrosine tyrosine, which also play a role in appetite suppression.

Ultimately it may turn out that different molecules may suit different patient populations and different conditions. 'It may be true that what is good for glucose homeostasis or what is good for losing weight may not be the best thing for chronic kidney disease,' suggests Kumar. 'There's going to be an explosion in just the sheer number of compounds and also the methods to make them.'

A hybrid approach

Gellman has taken a different approach to novel GLP-1 drugs based on his synthetic beta peptides. These are made by substituting some natural alpha amino acids with beta amino acids, that have the amino group attached to the beta carbon two atoms away from the carboxylate group. These artificial peptides or 'hybridtides', can form the same alpha helical structures as GLP-1, but are resistant to protease degradation. Gellman's company Longevity Biotech now has a drug candidate that activates both GLP-1 and GIP, is biased towards the insulin signalling pathway and can be orally formulated.

In his latest work Gellman has started to examine more closely how the membrane-anchored receptors engage with these drugs. He has found that a hybridtide with a kink near its end is able to wiggle between a helical and non-helical conformation within the receptor (both conformations being observed using cryo-electron microscopy). In doing so the molecule is constantly docking and undocking and lengthening the drug's action. 'I think most people think about these processes in terms of a single, ideal bound conformation of the peptide to the receptor as the basis for signalling,' says Gellman, 'but I'm increasingly suspecting that certain modes of dynamics are critical for signalling.' He is now trying to design this structural variability into his hybridtides to see if this will improve on the performance of GLP-1 drugs.

Getting to the brain

Trapp is working to fully understand how GLP-1 drugs work is still ongoing, particularly whether these peptide molecules penetrate the brain. A lot of clinicians think they do, but he is not persuaded. Rather, he thinks their ability to reduce appetite occurs by stimulation of parts of the brain that sit outside the blood–brain barrier – the selective semi-permeable membrane that keeps most large molecules out. His experiments with fluorescently labelled GLP-1 agonists prove this.

There are GLP-1 receptors and a second source of GLP-1 within the brain, completely isolated from the peripheral system and Trapp has shown that stimulating these receptors can have an even greater impact on weight loss in animal studies. Getting into the brain might also be important to treat neurodegenerative diseases where there are some promising results suggesting they slow disease progression. But targeting GLP-1 receptors in the brain will likely need a small molecule drug.

In fact several pharma companies already have small molecule GLP-1 agonists in their pipelines. 'Frankly, I was among the people who thought five years ago, there'll never be small molecules here, because the site you've got to bind is just too big,' says Gellman, but he concedes it looks like he was wrong. In 2023 Lilly published results of its phase 2 trial for orforglipron, a once-daily oral drug which achieved up to 14.7% mean weight reduction at 36 weeks, and Pfizer has completed phase 2 trial for its oral drug danuglipron and is now optimising the formulation.

If these oral small molecule drugs can match their larger cousins, they may solve the problem of the difficult mass production of peptide drugs. In the meantime, there has also been the first attempt to create a gene therapy that could integrate a GLP-1 secreting transgene directly into pancreas beta cells. In 2023, Fractyl Heath announced mice given semaglutide and treated with its gene therapy Rejuva, administered directly to the pancreas, had maintained a 22% weight loss for 28 weeks after stopping the drug and performed better than those given only semaglutide.

However the field develops, Trapp says the control of weight through GLP-1 is a genuine game-changer. 'Compared to what we had before, if we had weight loss of about 5%, that was a real success. Now, with these drugs, we're looking at 15%, and possibly even more.'

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https://chemistryworld.com

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Scientists develop new chemical tool for infection research

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Researchers from Würzburg and Berlin present a new molecule for visualizing the sphingomyelin metabolism. This offers prospects for innovative therapeutic approaches in infection research. The work is published in the journal Nature Communications.

At the end of the 19th century, German pathologist Ludwig Thudichum isolated previously unknown fatty substances (lipids) from the brain. He named the new class of molecules sphingolipids—after the Greek mythical creature Sphinx, out of respect for "the many riddles it posed to the researcher."

Since then, many diseases have been discovered that are caused by a faulty sphingolipid metabolism in the brain, including Fabry's disease and Gaucher's disease. Sphingolipids also have been connected to infectious diseases, for instance, viral infections with Ebola, measles or COVID-19, as well as bacterial infections with Pseudomonas aeruginosa or Staphylococcus aureus, which can cause middle ear infection, skin and lung infections and many other diseases.

In these infections, the degradation of the molecule sphingomyelin by the enzyme sphingomyelinase is often a crucial step. However, visualizing the enzyme's activity was previously impossible.

A new chemical probe to fill the gap

Researchers from Würzburg and Berlin have now succeeded in developing a sphingomyelin derivative that can be used to visualize the distribution of sphingomyelin and the activity of sphingomyelinase in infection processes.

The scientists are part of the Research Training Group 2581 "Metabolism, topology and compartmentalization of membrane proximal lipid and signaling components in infection." The chemists, physicists and biologists collaborated to synthesize novel chemical compounds and test their applicability in infection research.

"The new molecules are trifunctional sphingomyelins based on the natural product sphingomyelin and equipped with three additional functions. It was difficult to design such molecules that are accepted by the metabolism like its natural origin," says Professor Jürgen Seibel from

the Institute of Organic Chemistry at Julius-Maximilians-Universität (JMU) Würzburg in Bavaria, Germany.

Sphingomyelin degradation during development of Chlamydia bacteria imaged

The scientists demonstrated the function of their newly developed molecules not only by determining the activity of a bacterial sphingomyelinase on the surface of human cells, but they also visualized sphingomyelin degradation within human cells during the course of an infection with intracellular Chlamydia bacteria, which are known to infect the human genital tract and are suspected to contribute to the development of cancer in infected tissues.

Within their host cells, Chlamydia form a replicative organelle called an inclusion. The researchers showed that chlamydial inclusions mainly contain the cleaved forms of the trifunctional sphingomyelins.

Using so-called expansion microscopy and click-chemistry, they observed that the proportion of metabolized sphingomyelin molecules increased during the maturation of non-infectious to infectious Chlamydia particles. By being able to visualize this infection process, new targeted strategies against these infections can now be developed.

"The new chemical tool will certainly serve us well and can readily be used in many laboratories," Professor Seibel states. "Our aim is to use it to identify novel anti-infectious or immunotherapeutic strategies for drug development that can be used to combat infectious diseases by modulating sphingolipid metabolism."

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