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ASIA PACIFIC

Philippines releases draft regulations to amend requirements for designated establishments based on Energy Efficiency and Conservation Act

2023-08-18

On August 1, 2023, the Philippine Department of Energy (DOE) published three draft department circulars that stipulate compliance guidelines for various requirements for designated establishments in order to reclassify the designated establishments based on the Energy Efficiency and Conservation Act (RA11285) for each sector of industrial, commercial, and transport, and began soliciting opinions. Comments will be solicited until August 11, 2023. In addition to strengthening the threshold for designated establishments that are required to implement various energy efficiency and conservation measures, the draft department circulars stipulate the latest guidelines for the obligations on designated establishments, such as the submission of reports, the appointment of an Energy Efficiency (EE) Practitioner, and energy audits.

The details of the draft department circulars and the call for opinions can be viewed at the following URL:

https://www.doe.gov.ph/announcements/call-comments-three-3-draft-department-circular-designated-establishments-des-under

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Envilliance, 18-08-23

https://enviliance.com/regions/southeast-asia/ph/report_10760

Oversight of chemical restraint

2023-08-21

The Chief Psychiatrist will begin overseeing the use of chemical restraint from 1 September 2023.

From 1 September 2023 the Chief Psychiatrist will oversee the use of chemical restraint.

This is the first time that chemical restraint is being regulated in Victoria's mental health and wellbeing system.

Chemical restraint is defined as a restrictive intervention in the Mental Health and Wellbeing Act 2022.

It refers to the administration of a drug to a person for the primary purpose of controlling the person's behaviour by restricting their freedom of movement. Chemical restraint does not include the giving of a drug to a person for the purpose of treatment or medical treatment.

The use of chemical restraint by mental health and wellbeing services must be reported to the Office of the Chief Psychiatrist.

This reporting requirement will be implemented in stages, beginning with inpatient settings in designated mental health and wellbeing services on 1 September 2023.

In the subsequent period, the reporting requirement will be extended to all other settings where the new Act applies.

Further information on these changes and how to report chemical restraint is available in the the Chief Psychiatrist's Guideline on Restrictive Interventions.

Read More

Victoria Department of Health, 21-08-23

https://www.health.vic.gov.au/chief-psychiatrist/oversight-of-chemical-restraint

Proper implementation of laws a must to prevent air pollution in Dhaka

2023-08-23

Poor air quality in Bangladesh, particularly in Dhaka city, often makes global headlines. The capital city of the country has long been grappling with air pollution issues. Its air quality is usually unhealthy most days of the year.

Against this backdrop, experts on public health, policy analysts, rights activists and environmentalists have opined that if laws and rules related to air pollution control are implemented properly, the environment will improve. So, it is necessary to ensure the implementation of 'Air Pollution (Control) Rules, 2002'to prevent air pollution in Dhaka.

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Speaking at a discussion, they have called for proper implementation of 'Air Pollution (Control) Rules, 2022' and other relevant laws and regulations in order to prevent the air pollution in Dhaka city.

Bangladesh University of Health Sciences (BUHS), Center for Law and Policy Affairs (CLPA), Open Sesame and Japan Fund for Global Environment (JFGE) jointly arranged the discussion on 'Responsibilities to Improve Air Standard to Protect Public Health and Environment' at Ibrahim Auditorium of BUHS in the capital on Tuesday (August 22, 2023).

In addition to the 'Air Pollution (Control) Rules, 2022', it is also important to take initiatives to implement the air pollution prevention guidelines, said speakers of the discussion.

They also said that controlling air pollution will improve the environment as well as reduce disease and death. To ensure implementation of air pollution regulations, polluters need to be identified and punished according to law.

Professor Dr Md Anower Hussain, dean of Faculty of Public Health at Bangladesh University of Health Sciences (BUHS); presided over the discussion, while Professor Dr. Faridul Alam, vice-chancellor of BUHS, attended the event as the chief guest.

Read More

Bangladesh Post, 22-08-23

https://bangladeshpost.net/posts/proper-implementation-of-laws-a-must-to-prevent-air-pollution-in-dhaka-119038

AMERICA

Procedures for Chemical Risk Evaluation under TSCA

2023-08-14

As required under TSCA Section 6(b)(4), EPA published a final rule on July 20, 2017, that established a process for conducting risk evaluations to determine whether a chemical substance presents an unreasonable risk of injury to health or the environment, without consideration of costs or other non-risk factors, including an unreasonable risk to a potentially exposed or susceptible subpopulation, under the conditions of use. EPA states that this process incorporates the science requirements of the amended statute, including best available science and weight of the

scientific evidence. The final rule established the steps of a risk evaluation process, including: scope, hazard assessment, exposure assessment, risk characterization, and risk determination. EPA states that it is now considering revisions to that final rule and will solicit public comment through a notice of proposed rulemaking. EPA submitted a proposed rule to OMB for review on June 29, 2023. EPA intends to publish an NPRM in September 2023 and to issue a final rule in November 2024. More information on EPA's 2017 final rule is available in our June 26, 2017, memorandum.

Read More

The National Law Review, 14-08-23

https://www.natlawreview.com/article/epa-s-spring-2023-unified-agenda-includes-proposed-and-final-tsca-and-tri-rules

The Rubber Meets the Road with California's Green Chemistry Law

2023-08-17

- The California Department of Toxic Substances Control (DTSC) has designated motor vehicle tires containing the chemical N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) as a "priority product."
- The DTSC designation, which becomes effective on Oct. 1, 2023, makes tires containing 6PPD the seventh priority product identified under the state's Safer Consumer Products regulations.
- This Holland & Knight alert takes a closer look at the regulation's requirements for manufacturers of motor vehicle tires, as well as reviews related regulatory efforts and petitions by states and tribes.

What do nail polish, children's foam-padded sleeping mats and tires have in common? Not much at first glance, but all have been identified as "priority products" under California's Safer Consumer Products regulations administered by the California Department of Toxic Substances Control (DTSC) under the state's Green Chemistry law.

The Regulation and Its Requirements

The regulation designating motor vehicle tires containing the chemical N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine (6PPD) as a priority product became final on July 3, 2023, making tires containing 6PPD the seventh priority product identified under the law. DTSC's priority product

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designation for tires containing 6PPD will become effective on Oct. 1, 2023. As a result of the priority product designation, foreign and domestic manufacturers of motor vehicle tires whose products enter the stream of commerce in California will have until Nov. 30, 2023, to submit Priority Product Notifications to DTSC identifying those products. The notifications must be submitted through DTSC's online Safer Consumer Products Information Management System (CalSAFER).

Tires containing 6PPD subject to the regulation include those intended for use on light-duty vehicles (passenger cars, light trucks, vans and sport utility vehicles), motorcycles, motor homes, medium- and heavy-duty trucks, buses and trailers (including trailer coaches, park trailers and semitrailers). Significantly, tires containing 6PPD imported or sold into California as a component of a motor vehicle are excluded from the regulation, as are tires intended for use exclusively on off-road equipment, such as aircraft, construction, agricultural and industrial equipment, airport support equipment, ice grooming machines and military equipment. In addition, retread materials containing 6PPD are not covered.

Read More

Holland & Knight, 17-08-23

https://www.hklaw.com/en/insights/publications/2023/08/the-rubber-meets-the-road-with-californias-green-chemistry-law

Advocates Urge EPA Integration of Safer Chemicals and Organic Practices in Pesticide Assessments

2023-08-21

As the U.S. Environmental Protection Agency's (EPA) Safer Choice program asks for public input into the expansion of its work to label green chemicals, the need to recognize the importance of holistic management systems in sync with nature looms large. Will simple chemical substitution ignore the value of natural processes that require nurturing for sustainable future? EPA's Safer Choice is a non-regulatory program that identifies alternative chemicals for a number of uses that meet expanded safety criteria.

Tell EPA and Congress that substituting chemicals alone is not the Safer Choice. Use Safer Choice to eliminate harmful practices and emissions by compelling a transition to practices that build a climate- and sustainability-focused economy.

For problems requiring a chemical solution—for example, laundry detergents—EPA's Safer Choice is a valuable resource, and consumers can look for products with the Safer Choice label, which requires that EPA review all chemical ingredients that must meet safety criteria for both human health and the environment, including carcinogenicity, reproductive and developmental toxicity, toxicity to aquatic life, and persistence in the environment. While EPA's Safer Choice/Design for the Environment (DfE) program performs alternatives analyses on chemicals and identifies chemicals that are less hazardous, it stops short of identifying systems that make chemical inputs unnecessary. Substituting a less toxic pesticide, for example, is not the same as switching to available organic methods. [For pesticidal uses, the program is called Design for the Environment (DfE), which has so far been limited to disinfectants.]

Like Safer Choice, the National Organic Program (NOP) established by the Organic Foods Production Act (OFPA), is a label-centered program. Relying on consumer demand for food without pesticides or other chemical additives, produced in a way that benefits health, ecology, and biodiversity, NOP establishes standards for producers to use the organic label. OFPA does not require organic producers to use safer inputs. Rather, it requires them to adopt a system consistent with organic principles—building soil, increasing biodiversity, and producing healthy food—using only inputs that are natural (nonsynthetic) or are approved for a specific use by the National Organic Standards Board and placed into regulations on the National List. The growth of organic food sales in the U.S.—exceeding $60 billion in 2022—is based on consumer recognition of the value of organic food.

The organic program could have a larger impact if EPA, in its pesticide registration program, recognized that pesticide uses are unreasonable if the goals of the use could be met by available organic methods.

Read More

Beyond Pesticides, 21-08-23

https://beyondpesticides.org/dailynewsblog/2023/08/advocates-urge-epa-integration-of-safer-chemicals-and-organic-practices-in-pesticide-assessments/

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Revisions to Regulations on Persistent, Bioaccumulative, and Toxic (PBT) Chemicals Subject to TSCA

2023-08-14Y

TSCA directs EPA to take expedited action on certain PBTs to address the risks of injury to health or the environment presented by the chemical substance and to reduce exposure to the substance to the extent practicable. Consistent with that mandate, EPA issued final risk management rules restricting the use of five PBT chemicals in January 2021, and the rules went into effect in February 2021. EPA states that it is considering revisions to all five of the final rules to reduce further exposures, promote environmental justice, and better protect human health and the environment. EPA submitted a proposed rule to OMB for review on July 21, 2023. EPA intends to publish an NPRM in October 2023. More information on EPA's PBT rules is available in our September 3, 2021, memorandum.

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The National Law Review, 14-08-23

https://www.natlawreview.com/article/epa-s-spring-2023-unified-agenda-includes-proposed-and-final-tsca-and-tri-rules

EPA: PFAS drinking water crisis worse than previously reported

2023-08-18

- Water utility data submitted to the agency shows hundreds of new detections of "forever chemicals" in water.
- The Biden administration must this year urgently finalize its national drinking water standards for tackling PFAS.

WASHINGTON – Today the Environmental Protection Agency revealed that 26 million people in hundreds of communities have the toxic "forever chemicals" known as PFAS in their drinking water.

The EPA's Fifth Unregulated Contaminant Monitoring Rule, or UCMR5, requires water utilities across the nation to test drinking water for 29 different PFAS compounds.

The initial round of data that the agency released today confirms the presence of PFAS at 431 water systems at levels above minimum reporting

limits. This is consistent with a 2020 study published by scientists at the Environmental Working Group that estimated more than 200 million Americans could have PFAS in their drinking water.

"For decades, millions of Americans have unknowingly consumed water tainted with PFAS," said Scott Faber, senior vice president for government affairs at EWG.

"The new testing data shows that escaping PFAS is nearly impossible. The EPA has done its job, and the Biden White House must finalize drinking water standards this year," Faber added.

EWG's interactive map now shows public and private water systems known to be contaminated with toxic PFAS at more than 2,800 locations in 50 states, the District of Columbia and two territories. The true scale of PFAS contamination is expected to be much greater.

The new UCMR5 data will soon be added to the PFAS Map.

More UCMR5 testing for PFAS will take place between 2023 and 2025, with new data expected quarterly. EPA collects data through the UCMR for contaminants suspected to be in drinking water and for which Safe Drinking Water Act, or SDWA, health-based standards do not exist.

Read More

EWG, 18-08-23

https://www.ewg.org/news-insights/news-release/2023/08/epa-pfas-drinking-water-crisis-worse-previously-reported

Significant New Use Rules (SNUR) for Certain Non-Ongoing Uses

2023-08-14

EPA states that it is authorized to designate a particular new use (or return of a phased-out use) of a chemical substance as a "significant new use" under TSCA Section 5(a)(2) by rule after consideration of relevant factors. EPA would use these rules to require notice to EPA before chemical substances and mixtures are used in new ways that might create concerns. Persons subject to the SNUR who intend to manufacture (including import) or process the chemical substance for the significant new use must notify EPA at least 90 days prior to initiating activities via a significant new use notice (SNUN). EPA is developing TSCA Section 5(a)(2) SNURs on conditions of use identified as not currently ongoing in the final scope

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documents for the following High Priority Substances undergoing TSCA Section 6 risk evaluations:

- Other Chemical Substances Undergoing Risk Evaluation under TSCA (RIN: 2070-AL05): Although EPA intended to publish an NPRM in June 2023, it has not published anything to date. EPA intends to issue a final rule in May 2024.
- Phthalates (RIN: 2070-AL06): Although EPA intended to publish an NPRM in June 2023, it has not published anything to date. EPA intends to issue a final rule in June 2024.
- Flame Retardants (RIN: 2070-AL07): EPA published an NPRM in June 2023 and intends to issue a final rule in May 2024. More information on the NPRM is available in our July 3, 2023, memorandum.
- Certain Solvents (RIN: 2070-AL08): Although EPA intended to publish an NPRM in June 2023, it has not published anything to date. EPA intends to issue a final rule in May 2024.

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The National Law Review, 14-08-23

https://www.natlawreview.com/article/epa-s-spring-2023-unified-agenda-includes-proposed-and-final-tsca-and-tri-rules

EUROPE

Update on smoke-free environments recommendation

2023-08-16

To be presented by Commission by the end of 2023

As part of its work programme for 2023, the European Commission announced an update of the Council Recommendation on smoke-free environments from 2009. The proposal, which will be published by the end of the year, is part of Europe's Beating Cancer Plan.

According to the European Commission, the update of the current Council recommendation will introduce the objective of protecting people across the EU from exposure to second-hand smoke by extending its coverage to emerging products, such as e-cigarettes and heated tobacco products, and by expanding smoke-free environments, including outdoor spaces like schools and playgrounds.

According to the World Health Organisation (WHO), Europe has the highest prevalence of tobacco smoking among adults at 28%.

The European Commission's plan aims to create a 'Tobacco-Free Generation' by 2040, with less than 5% of the population using tobacco.

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Euractiv, 16-08-23

https://www.euractiv.com/section/health-consumers/news/show-must-go-on-for-eu-health-policy-after-summer/

Fast food: PFAS pollutants in packaging

2023-08-22

How to make cardboard packaging for burgers and fries' grease resistant? By using PFAS, these perfluorinated substances whose toxicity is now widely denounced. They are ubiquitous in fast food packaging used in France, according to a new study published on August 4, 2023, and conducted by Spanish researchers and Jacob de Boer, a Dutch specialist in the subject. Future Generations, which reveals these results, had already pointed out this problem with several European NGOs in 2021.

Between September and November 2021, the researchers collected forty-seven packages containing fries, hamburgers, or other nuggets, from various fast-food restaurants. They searched for forty perfluorinated compounds, including well-known long-chain PFAS (PFOA, PFOS) but also shorter-chain PFAS and precursors.

Read More

Reporterre, 22-08-23

https://reporterre.net/Fast-food-des-polluants-PFAS-dans-les-emballages

List of critical medicines

2023-08-16

The Commission is to present a list of critical medicines that will include drugs considered essential for health systems at the EU level as a countermeasure for drug shortages.

Kyriakides announced that the list would be presented by the end of the year and would help "monitor the availability of essential medicines and address supply chain vulnerabilities".

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The list will not be linked to an EU stockpiling system for essential medicines, which the Commission reserves the right to create if needed.

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Euractiv, 16-08-23

https://www.euractiv.com/section/health-consumers/news/show-must-go-on-for-eu-health-policy-after-summer/

Ambient Air Quality Directives

2023-08-16

In September's plenary session in Strasbourg, the European Parliament is set to adopt a text on Ambient Air Quality Directives.

This comes as part of the European Green Deal's zero pollution ambition after a proposal from the European Commission published in 2022.

Following this proposal, the Parliament's health committee (ENVI) adopted a report in June that aims for a cleaner and healthier environment by setting strict rules for several pollutants, including nitrogen dioxide (NO2), sulphur dioxide (SO2) and ozone (O3).

The text also reinforces the 2030 limit and proposes that national authorities create an air quality roadmap to set up measures to comply with the new rules.

The Parliament and the Commission stress the need for future reviews to comply with the WHO guidelines.

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Euractiv, 16-08-23

https://www.euractiv.com/section/health-consumers/news/show-must-go-on-for-eu-health-policy-after-summer/

A bit more on chemicals: F-gases and PFAS

2023-08-16

The ongoing debate over F-gases…

EU law to phase out fluorinated gases, also known as F-gases, remains on the table as Parliament and Council failed to seal the deal during a session on 19 July.

F-gases have medical applications in inhalation anaesthetics and metered dose inhalers (MDIs), a type of inhaler used to treat asthma and chronic obstructive pulmonary disease.

More climate-friendly alternatives are not easy to find for all F-gases applications, particularly for medical ones. Therefore, MEPs in the Commission's proposal included amendments on the participation of the European Medicines Agency (EMA) in coordinating the approval process of replacing fluorinated substances in pharmaceutical products.

…in the meantime PFAS

Five EU countries – Denmark, Germany, the Netherlands, Sweden and Norway – on 13 January submitted a restriction proposal to the European Chemicals Agency (ECHA) on over 10,000 per- and poly-fluoroalkyl substances (PFAS) under the REACH regulation.

Due to the broad ban, it is also known as a universal PFAS restriction, which aims to address the risks to the environment and human health from the manufacture, placing on the market and using PFAS.

Currently, a six-month consultation on the proposal is open until 25 September 2023. Simultaneously the proposal is undergoing an independent scientific assessment in the European Chemicals Agency (ECHA) Committees. At the next ECHA's committees meeting with Commission in September, it is planned look at hazard assessment and different sectors where PFAS are used.

This is not the first take on PFAS – under the EU's chemicals strategy, the Commission is committed to phasing out the use of PFAS in the EU unless their use is essential for society.

There are several PFAS already banned under REACH. Additionally, a restriction proposal for perfluorohexane-1-sulphonic acid (PFHxS) is in the advanced stages and is hoped to be adopted by the end of this year or early next year.

Another restriction proposal regards firefighting foams which, in terms of emissions into the environment, are a major source of PFAS. ECHA finalised its opinion, and now the Commission has to decide on the restriction together with the member states.

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Euractiv, 16-08-23

https://www.euractiv.com/section/health-consumers/news/show-must-go-on-for-eu-health-policy-after-summer/

Approach on chemicals to be unveiled in the last quarter of 2023

2023-08-16

Another file the Commission has been late in presenting is the revision of the chemical safety law – the Regulation on the Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) – which was initially due to be presented by the end of 2022 but is now due in the fourth quarter of this year.

According to the European Environmental Bureau (EBB), Commissioners decided to delay it following pressure from the German chemicals industry. Campaigners worried in February that Commission President Ursula von der Leyen would seek to please her political base in Germany with a softball approach to chemicals regulation.

The worries seemed fair as the Commission could be about to cave to industry pressure over its initial plans to ban certain toxic chemicals under its chemicals strategy, a leaked document seen by EURACTIV in July suggests.

The strategy included banning the most harmful chemicals in consumer products, such as toys, cosmetics, detergents, food contact materials and textiles, through revising the law REACH.

But according to the leak seen by EURACTIV, the Commission is slashing its ambition to between 1% and 50% of chemicals, a significant decrease from the previous strategy.

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Euractiv, 16-08-23

https://www.euractiv.com/section/health-consumers/news/show-must-go-on-for-eu-health-policy-after-summer/

New task for ECHA to make batteries safer

2023-08-17

ECHA/NR/23/20

ECHA will support the European Commission in identifying substances of concern found in batteries or used in their manufacturing. It will also prepare proposals to restrict substances in batteries. The aim is to make batteries on the EEA market more sustainable throughout their lifecycle.

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Helsinki, 17 August 2023 – With the modernisation of the EU's regulatory framework for batteries, ECHA has received new tasks to support the European Commission. The Agency will assist in the development of a Commission report into substances of concern found in batteries or used in their manufacturing, that have negative impacts on human health, the environment or recycling for safe and high-quality raw materials.

The report, expected by 31 December 2027, will identify the substances and consider follow-up measures, such as possible Union-wide restrictions. It is expected that ECHA will begin its work toward this report in 2024.

Additionally, the Commission may request ECHA to prepare restriction proposals on harmful substances in batteries and waste batteries. The Agency will also provide an opinion, through its committees for Risk Assessment and Socio-Economic Analysis, on the restriction proposal's effectiveness in managing the risk and its impact on society.

Background

The Regulation (EU) 2023/1542 of the European Parliament and of the Council of 12 July 2023 concerning batteries and waste batteries, amending Directive 2008/98/EC and Regulation (EU) 2019/1020 and repealing Directive 2006/66/EC entered into force on 17 August 2023.

Read More

ECHA, 17-08-23

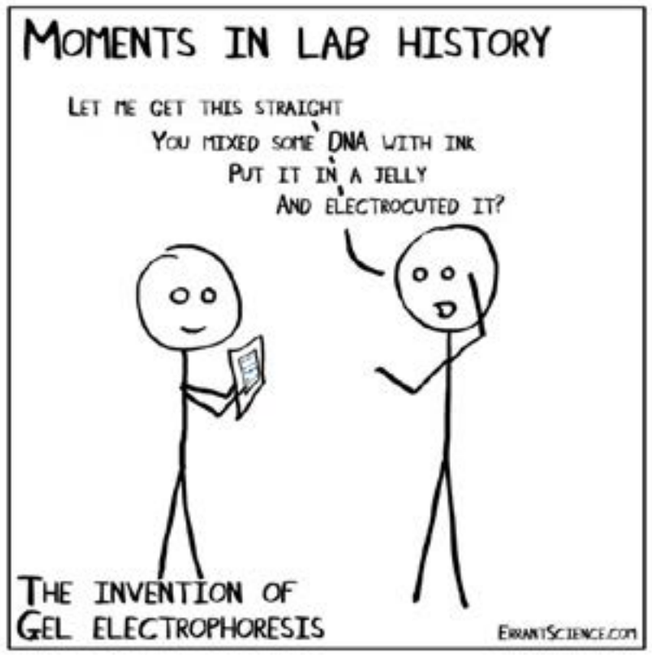
https://echa.europa.eu/-/new-task-for-echa-to-make-batteries-safer

Janet's Corner

SEP. 01, 2023

Sometimes science is actually just mixing stuff up!

2023-09-01



https://twitter.com/ErrantScience/status/1642435591336755200

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Hazard Alert

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Allyl Chloride

2023-09-01

USES [2,3]

Allyl chloride is used as a chemical intermediate in the manufacture of pharmaceuticals, varnishes, epoxy resins, adhesives, plastics, gylcerol, and insecticides. [3] Almost all of the allyl chloride produced is used to make epichlorohydrin and glycerin. In addition, it is used in the synthesis of allyl compounds such as allyl alcohol, allyl amines, allyl esters, and polyesters.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- Possible sources of allyl chloride emissions to the ambient air are production and processing facilities.
- Occupational exposure exists for people working in the production of allyl chloride, epichlorohydrin, and synthetic glycerin.
- Individuals may be exposed to allyl chloride through breathing contaminated air or through skin contact.

Routes of Exposure

The main routes of exposure to allyl chloride are:

- Inhalation;
- Skin absorption;
- Ingestion;
- Skin and/or eye contact

HEALTH EFFECTS [4]

Acute Health Effects

- Acute inhalation exposure to high levels of allyl chloride in humans has resulted in irritation of the eyes and respiratory passages and unconsciousness.
- Intense exposure also produces conjunctivitis, reddening of eyelids, and corneal burn.
- Acute animal tests in rats, mice, and guinea pigs, have shown allyl chloride to have moderate toxicity from oral and inhalation exposure.

Allyl chloride is the organic compound with the molecular formula C3H5Cl. [1] It is a colourless, light yellow or amber liquid with an unpleasant pungent odour. It is highly flammable. [2] Allyl chloride is slightly soluble in water and miscible with alcohol, chloroform, ether, and petroleum ether. In the United States, allyl chloride is a federal hazardous air pollutant and was identified as a toxic air contaminant in April 1993. [1,2]

Carcinogenicity

- No human cancer data were located for allyl chloride.
- Limited animal studies indicate that exposure to allyl chloride by gavage (placing the chemical experimentally in the stomachs of mice) caused an increase in the incidences of a rare forestomach tumour. Similar skin painting studies produced site specific tumours.
- Allyl chloride is an alkylating agent and structurally related to probable human carcinogens.
- EPA considers allyl chloride to be a possible human carcinogen (cancer-causing agent) and has ranked it in EPA's Group C.
- EPA has not calculated an inhalation unit risk estimate for allyl chloride.
- The California Environmental Protection Agency (CalEPA) has established an inhalation unit risk estimate of 6.0 x 10-6 (µg/m3)-1 and an oral cancer slope factor of 2.1 x 10-2 (mg/kg/d)-1 for allyl chloride.

Other Effects

- Limited human data were considered inadequate in providing evidence of reproductive or developmental effects in humans exposed to allyl chloride.
- One animal study involving the inhalation of allyl chloride in rabbits resulted in decreased maternal weight gain.
- Rats that were injected with allyl chloride had increased maternal heart, liver, spleen and kidney weights.

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. Cold water may be used. WARM water MUST be used. 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 immediate medical attention.

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- **Inhalation**: If inhaled, remove to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical attention immediately.
- **Serious Inhalation**: Evacuate the victim to a safe area as soon as possible. Loosen tight clothing such as a collar, tie, belt or waistband. If breathing is difficult, administer oxygen. If the victim is not breathing, perform mouth-to-mouth resuscitation. WARNING: It may be hazardous to the person providing aid to give mouth-to-mouth resuscitation when the inhaled material is toxic, infectious or corrosive. Seek immediate 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:

- Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapours below their respective threshold limit value.
- Ensure that eyewash stations and safety showers are proximal to the work-station location.

Personal Protective Equipment [5]

The following personal protective equipment is recommended when handling allyl chloride:

- Splash goggles;
- Lab coat;
- Vapour respirator (be sure to use an approved/certified respirator or equivalent);
- Gloves.

Personal Protection in Case of a Large Spill:

- Splash goggles;
- Full suit;
- Vapour respirator;
- Boots;
- Gloves;

- A self contained breathing apparatus should be used to avoid inhalation of the product.
- Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

REGULATION

United States

NIOSH: The National Institute for Occupational Safety & Health has established a Relative Exposure Limit (REL) for allyl chloride of:

Time Weighted Average concentration of 1 ppm (3 mg/m3)

Short term exposure concentration of 2 ppm (6 mg/m3)

OSHA: The Occupational Safety & Health Administration has set a Permissible Exposure Limit (PEL) for allyl chloride of: TWA 1 ppm (3 mg/m3)

ACGIH: the American Conference of Governmental Industrial Hygienists has set a time weighted average Threshold Limit Value (TLV) for allyl chloride of: 3mg/m3

Australia

Safe Work Australia: Safe Work Australia has established a time weighted average concentration of allyl chloride of:

- (3mg/m3) for an 8 hour work day
- 2ppm (6mg/m3) 15 minute short term exposure limit

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Scientists use quantum device to slow down simulated chemical reaction 100 billion times

2023-08-28

Joint lead researcher and Ph.D. student, Vanessa Olaya Agudelo, said, "It is by understanding these basic processes inside and between molecules that we can open up a new world of possibilities in materials science, drug design, or solar energy harvesting.

"It could also help improve other processes that rely on molecules interacting with light, such as how smog is created or how the ozone layer is damaged."

Specifically, the research team witnessed the interference pattern of a single atom caused by a common geometric structure in chemistry called a "conical intersection."

Conical intersections are known throughout chemistry and are vital to rapid photo-chemical processes such as light harvesting in human vision or photosynthesis.

Chemists have tried to directly observe such geometric processes in chemical dynamics since the 1950s, but it is not feasible to observe them directly given the extremely rapid timescales involved.

To get around this problem, quantum researchers in the School of Physics and the School of Chemistry created an experiment using a trapped-ion quantum computer in a completely new way. This allowed them to design and map this very complicated problem onto a relatively small quantum device—and then slow the process down by a factor of 100 billion. Their research findings are published August 28 in Nature Chemistry.

"In nature, the whole process is over within femtoseconds," said Olaya Agudelo from the School of Chemistry. "That's a billionth of a millionth—or one quadrillionth—of a second.

"Using our quantum computer, we built a system that allowed us to slow down the chemical dynamics from femtoseconds to milliseconds. This allowed us to make meaningful observations and measurements.

"This has never been done before."

Joint lead author Dr. Christophe Valahu from the School of Physics said, "Until now, we have been unable to directly observe the dynamics of 'geometric phase'; it happens too fast to probe experimentally.

Scientists at the University of Sydney have, for the first time, used a quantum computer to engineer and directly observe a process critical in chemical reactions by slowing it down by a factor of 100 billion times.

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"Using quantum technologies, we have addressed this problem."

Valahu said it is akin to simulating the air patterns around a plane wing in a wind tunnel.

"Our experiment wasn't a digital approximation of the process—this was a direct analog observation of the quantum dynamics unfolding at a speed we could observe," he said.

In photo-chemical reactions such as photosynthesis, by which plants get their energy from the sun, molecules transfer energy at lightning speed, forming areas of exchange known as conical intersections.

This study slowed down the dynamics in the quantum computer and revealed the tell-tale hallmarks predicted—but never before seen—associated with conical intersections in photochemistry.

Co-author and research team leader, Associate Professor Ivan Kassal from the School of Chemistry and the University of Sydney Nano Institute, said, "This exciting result will help us better understand ultrafast dynamics—how molecules change at the fastest timescales.

"It is tremendous that at the University of Sydney we have access to the country's best programmable quantum computer to conduct these experiments."

The quantum computer used to conduct the experiment is in the Quantum Control Laboratory of Professor Michael Biercuk, the founder of quantum startup, Q-CTRL. The experimental effort was led by Dr. Ting Rei Tan.

Tan, a co-author of the study, said, "This is a fantastic collaboration between chemistry theorists and experimental quantum physicists. We are using a new approach in physics to tackle a long-standing problem in chemistry."

Phys Org, 28 August 2023

https://phys.org

A first for ferrocene: Organometallic capsule with unusual charge-transfer interactions

2023-08-29

Simply put, one can make ferrocene-based compounds reversibly switch between different oxidation states by changing the conditions of their

Ferrocene is an emergent organic-metal hybrid compound, and its accidental discovery has led to the rapid development of organometallic chemistry. Aside from its interesting structure, which consists of an iron atom sandwiched between two pentagonal organic rings, ferrocene has remarkable redox-responsive properties.

redox environment, which essentially dictates how electron transfers occur between molecules. Although the properties of ferrocene-based compounds could be very useful in materials science, drug delivery, and catalysis, there are almost no known methods to facilely and precisely synthesize multi-ferrocene-based capsules with more than five ferrocene units.

Fortunately, a research team from Tokyo Institute of Technology in Japan has found a solution to this problem. In their latest study, which was conducted by Kazuki Toyama (doctoral student), Assistant Professor Yuya Tanaka, and Professor Michito Yoshizawa, and published in Angewandte Chemie International Edition, the researchers found an ingenious way to prepare a ferrocene-based capsule with unusual properties.

The key to the synthesis of the capsule is a ferrocene-containing amphiphile, which the researchers referred to as "FA". Each FA molecule consists of two hydrophobic ferrocene groups bound to a meta-phenylene ring, which is also connected to two hydrophilic trimethylammonium groups. The bent hydrophobic framework and its hydrophobic effect cause multiple FA molecules to quickly and spontaneously assemble into organometallic capsule (FA)n in water.

Interestingly, the capsule can be reversibly disassembled and assembled by providing appropriate chemical stimuli. For example, adding an oxidant such as iron chloride to water containing (FA)n leads to the immediate disassembly of the capsule. Moreover, the subsequent addition of a reductant such as ascorbic acid neutralizes the oxidant, leading to the quick reassembly of the capsule.

The on-demand assembly and disassembly of the new capsule becomes even more useful when considering that it can bind to guest molecules in the cavity. The researchers found that capsule (FA)n is a more versatile host than previous ones, as Toyama says, "In contrast to previous multi-ferrocene compounds, the present capsule efficiently encapsulates typical organic and inorganic dyes, such as perylenetetracarboxylic diimide and copper-phthalocyanine, as well as electron-accepting molecules, such as chloranil and tetracyanoquinodimethane, in water."

The team discovered unusual host-guest charge-transfer interactions upon the encapsulation of electron-accepting molecules by the capsule (FA)n. The interactions were observed as relatively wide absorption bands, ranging from 650-1350 nm, in the visible to near-infrared spectrum. These interactions could also be reversibly turned on and off by controlling the assembly and disassembly of the capsule.

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The present multi-ferrocene-based capsule could find applications across various fields, such as medicine, biotechnology, chemical synthesis, and more. Further studies are already underway. "On the basis of the present achievement, our next study will focus on the development of various types of organometallic capsules, such as ones with magnetic and medicinal properties and catalytic activity," concludes Dr. Tanaka.

Phys Org, 29 August 2023

https://phys.org

New bioink promotes growth & regeneration of 3D-printed muscle tissue

2023-08-29

Researchers have developed a novel bioink that uses a sustained-release hormone to promote the growth and regeneration of 3D-printed muscle tissues. Their approach opens the door to developing new therapies to help people who've suffered muscle loss or damage due to trauma, disease, or surgery.

Generating native-like muscle tissue can be a tricky business. The tissue consists of many different cell types, and the environment around muscles is regulated by complex biochemical and biomechanical pathways, including inflammatory cytokines and growth factors that maintain internal stability and support tissue repair.

Currently, repairing muscles injured or lost because of trauma, disease, or surgery involves transferring healthy muscle to the affected site, a technique called autologous transfer. This isn't ideal as it negatively impacts the area from which the healthy tissue is taken, and complications such as poor innervation can impede functional muscle recovery.

Now, researchers from the Terasaki Institute for Biomedical Innovation (TIBI) in Los Angeles have come up with a novel, improved bioink to enhance 3D-printed skeletal muscle constructs and overcome the limitations of autologous transfer.

Normal skeletal muscle development is a gradual process that relies on myoblasts, committed muscle cell precursors, fusing together to form myotubes, which eventually become muscle fibers. This process is called myogenesis. So, in engineering muscles, it's crucial that functionality is maintained by ensuring maturing muscle cells are structurally aligned and their survivability is enhanced.

To mimic myogenesis, the researchers relied on a key ingredient in their specially formulated bioink: insulin-like growth factor-1 (IGF-1), a hormone with a molecular structure similar to insulin that, along with growth hormone, is vital for normal bone and tissue growth and development.

The bioink is composed of a biocompatible gelatin-based hydrogel called gelatin methacryloyl (GelMA), myoblast cells, and PLGA microparticles coated with IGF-1 designed to slowly release the hormone as the particles degraded. Poly(lactic-co-glycolic acid) or PLGA is one of the most effective biodegradable polymeric nanoparticles due to its sustained-release properties, low toxicity and biocompatibility. A control version of the bioink was created without IGF-1.

The researchers found that three days after bioprinting muscle constructs, the myoblasts were viable, confirming that the printing process had not damaged the cells. They observed enhanced myoblast alignment and the fusion of myoblasts to form myotubes, which were significantly longer and wider in the constructs containing IGF-1. Myotubes covered 25% of the area in the PLGA/IGF-1 condition, compared to less than 16% in the control condition.

At around 10 days after bioprinting, the formed tissue started to contract spontaneously with enough force that it shook the hydrogel substrate, as seen in the video below. The amplitude of the contractions was significantly higher in areas incorporating the sustained release of IGF-1.

The researchers then implanted 3D-printed muscle constructs into mice. After six weeks, the mice that received the constructs with sustained-release IGF-1 showed the most muscle tissue regeneration. They concluded that the study's findings strongly suggested that their novel bioink allowed the development of a contractile 3D structure closely resembling native muscle tissue.

"The sustained release of IGF-1 facilitates the maturation and alignment of muscle cells, which is a crucial step in muscle tissue repair and regeneration," said Ali Khademhosseini, corresponding author of the study. "There is great potential for using this strategy for the therapeutic creation of functional, contractile muscle tissue."

The study was published in the journal Macromolecular Bioscience.

New Atlas, 29 August 2023

https://newatlas.com

Meta-analysis results call into question the efficacy of paroxetine for hot flashes.

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Benefits of Drug for Hot Flashes Are Comparable to Placebo, Meta-Analysis Suggests

2023-08-30

Hot flashes are one of the most concerning and most reported symptoms among menopausal women and breast cancer survivors. Currently, paroxetine is a FDA-approved non-hormonal drug used for the treatment of hot flashes. In an article published this month in the journal Frontiers in Psychiatry, researchers at Baylor University tested the efficacy of paroxetine by conducting a systematic review and meta-analysis of six clinical trials, finding that the benefits of paroxetine in the treatment of hot flashes to be comparable to that of the placebo response.

The study included information from all available clinical trials of paroxetine for hot flashes and provides the most comprehensive view of the drug's benefits.

"This is the first meta-analysis to systematically review clinical trials of paroxetine versus placebo with the aim of determining the magnitude of the placebo response among included clinical trials," said Joshua Rhodes, Ph.D. ('23), research assistant and lead author. "It is also the most robust with the inclusion of both published and unpublished outcome data derived from the national clinical trial database."

In clinical trials of treatments for hot flashes, the drug or other intervention is usually compared to a placebo (such as a "sugar pill" or non-effective intervention). This helps to determine if a medication has actual effects or if the perceived benefits are due to other factors such as having a hope or expectancy of benefit. Since paroxetine is used by many women, it is very important to have information about the effects beyond taking a placebo pill. The Baylor study was conducted to examine the extent of such placebo factors in taking paroxetine for hot flashes.

The researchers coded and analyzed the six randomized clinical trials that included 1,486 women. The results demonstrated that the placebo response accounted for the majority of treatment responses for reductions in both hot flash frequency and severity:

79% of the mean treatment response for hot flash frequency is accounted for by a placebo response, resulting in a mean true drug effect of 21% at most.

Additionally, 68% of the mean treatment response for hot flash severity is accounted for by a placebo response, resulting in a maximum true drug effect of 32%.

"We sought to provide objective information for women about the actual active drug benefit of taking paroxetine for hot flashes," said Gary Elkins, Ph.D., professor of psychology and neuroscience and director of the Mind-Body Medicine Research Laboratory at Baylor. "Our intent is to provide information that is needed for women to make informed decisions about taking paroxetine and the benefit beyond the non-specific effects of placebo."

Paroxetine efficacy

The drug paroxetine mesylate, marketed under the trade name of Brisdelle, is an SSRI used to treat anxiety and depression with associated potential side effects, including headache, fatigue, nausea/vomiting and a specific warning for increased risk of suicidal ideation.

"Results indicated that most of the benefit of paroxetine in reducing hot flashes is due to a non-specific placebo response. The meta-analysis shows that the benefit is rather small and is mostly due to placebo effects rather than drug-specific effects," Elkins said. "Further, this antidepressant medication has undesirable side effects and may reduce the benefit of breast cancer preventive medications."

Although the results call into question the efficacy of paroxetine for hot flashes, more research is needed to reevaluate the use of paroxetine to treat postmenopausal hot flashes and and emphasize the importance of considering effective, alternative treatments, the researchers said.

Reliable treatment needed for hot flashes

Hot flashes are triggered by a decline in estrogen either during natural menopause or as a result of breast cancer treatments. Approximately 80% of menopausal women and about 96% of breast cancer survivors experience hot flashes to some degree. For those experiencing these symptoms, it can cause a marked decrease in quality of life, physical discomfort and sleep disturbances. Symptoms generally last about seven years on average but can continue for 20 or more years for some women, Elkins said.

Previously, hormone replacement therapy (HRT) was widely used to manage hot flashes. However, research has shown that HRT is associated with an increased risk of breast cancer and cardiovascular disease for some

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women. Because of this, women often search for alternative solutions for symptom relief.

Having as much accurate information as possible about HRT and alternatives such as paroxetine empowers women to make decisions about how best to manage hot flashes and symptoms associated with menopause, Elkins said. The Baylor study provides important information for healthcare providers and women with menopausal symptoms who desire to avoid HRT for hot flashes.

The findings emphasize the need for more research to determine alternative and integrative health interventions for hot flashes, e.g., hypnotherapy, mindfulness, medications, and to address women's health concerns.

Reference: Rhodes JR, Alldredge CT, Elkins GR. Magnitude of placebo response in clinical trials of paroxetine for vasomotor symptoms: a meta-analysis. Front Psychiatry. 2023;14. doi: 10.3389/fpsyt.2023.1204163

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Technology Networks, 30 August 2023

https://technologynetworks.com

One-pot synthesis of iron–sulfur proteins under aerobic conditions

2023-08-29

These clusters are of keen research interest since they are considered to be a critical part of evolution. They serve as a link between pre-biotic chemistry (chemical processes that existed prior to the emergence of life forms) and the complex molecular and biological systems we know today. Put simply, they might be one of the primitive catalysts that led to the emergence of life on Earth. Thus, having convenient methods to synthesize Fe–S proteins will hopefully advance our understanding of young Earth biology and help us answer the ultimate question of the origin of life.

However, despite their prevalence, the synthesis of mature Fe–S proteins outside the cell has proven to be challenging. They not only require intricate cellular machinery for synthesis but also degrade easily upon contact with oxygen due to its reaction with their Fe–S clusters.

S clusters, which are a part of Fe–S proteins, are found across all forms of life. They play a significant role as biological cofactors—helper molecules that assist these proteins in different biochemical trans-formations—that are involved in respiration and metabolism.

Therefore, scientists had been forced to follow the complicated route of first producing and extracting an incomplete (or 'apo') protein, followed by its maturation (addition of the Fe–S cofactor) under strictly oxygen-deprived conditions. But what makes this process even harder is the presence of contaminating iron-containing proteins in the final extract.

A team of researchers, including Associate Professors Kosuke Fujishima and Shawn McGlynn from the Earth-Life Science Institute (ELSI), Tokyo Institute of Technology and Assistant Professor Po-Hsiang Wang from the National Central University have developed a novel protocol for producing mature [4Fe-4S] proteins in which the Fe–S cluster is placed within a cube-like structure.

The team devised a specialized Fe–S assembly protein system pathway that would function in an oxygen-free environment due to the presence of an oxygen-scavenging system to deliver mature Fe–S proteins. The paper is published in the journal ACS Synthetic Biology.

The researchers first sought to assemble what's known as the sulfur formation (SUF) system. In bacteria, this multi-protein system contains all the necessary machinery to produce [4Fe-4S] clusters. It has a higher tolerance for oxygen when compared to the other pathways with similar functions (such as nitrogen fixation and the iron–sulfur cluster system). The research team created a recombinant SUF pathway that consists of six protein subunits with the ability to function in a cell-free environment.

In order to maintain an oxygen-free environment within the test tube, the researchers then introduced a three-enzyme cascade (a set of three enzymatic reactions that occur in a sequence) that serves as an oxygen-scavenging system. While this scavenging system removes oxygen from the environment, it also improves the efficiency of the system. It achieves this by producing reduced flavin adenine dinucleotide (FADH2), an electron-carrier which is needed for the synthesis of Fe-S cluster by SUF system.

Finally, for the synthesis of apo protein, the team adopted a specialized cell-free method that enables the in vitro production of proteins by using reconstituted cell-free protein synthesis known as PURE system. With the addition of genetic material (DNA or mRNA) and the necessary sources of energy, the PURE system essentially acts as an artificial protein factory.

Thus, the researchers combined the PURE system, the O2-scavenging enzyme cascade, and the components of the SUF pathway in a single

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tube to perform one-pot, cell-free synthesis of two representative [4Fe-4S] proteins: aconitase and thermophilic ferredoxin.

Explaining the iterative processes experienced in getting the pieces of the puzzle to fit together, a co-first author Ph.D. student Shota Nishikawa comments, "It was challenging to home-on to the appropriate stoichiometry and substrate/cofactor concentration. Nevertheless, we performed thorough studies to characterize the proper ratio of enzymes needed in the PURE system."

The protocol developed in this study has significant implications for the scientific community. "We have created a novel and convenient method for the synthesis of mature Fe–S proteins which no longer requires a bulky glove box," says Fujishima. He claims that their protocol overcomes the traditional challenges of the [4Fe–4S] cluster assembly and O2 sensitivity, which have been major obstacles in the fields of synthetic biology and anaerobic enzymology.

By greatly extending the capabilities of the PURE system, the strategy proposed by the researchers could lead to the development of new biotechnologies and a better understanding of the fundamentals of protein synthesis and assembly.

With eyes on the future, the researchers note that this work opens several doors for upcoming studies. Being able to implement in vitro oxygen-free environments could help scientists replicate other types of multi-protein pathways, such as the nitrogen fixation (NIF) andiron–sulfur cluster (ISC) pathways, to synthesize other metal cofactor-bearing enzymes. This, in turn, may lead to the development of new biocatalysts and synthetic cells, with potential applications in environmental remediation, energy production, medicine, and astrobiology.

Phys Org, 29 August 2023

https://phys.org

Paper straws not so eco-friendly, 90% contain toxic "forever chemicals"

2023-08-24

"Forever chemicals" is the colloquial name given to a class of more than 12,000 chemicals, more formally known as poly- and perfluoroalkyl substances (PFAS), that barely break down in the environment or in our bodies. Hence, the "forever" part.

A new European study has found that 90% of so-called eco-friendly paper straws contain "forever chemicals," compounds that don't – or barely – break down and can accumulate in our bodies, leading to health problems. The findings are consis-tent with results from a recent US study.

Humans are mainly exposed to PFAS through food and drinking water. In addition, many food packaging materials and plastic bags can also contain PFAS, which can be transferred to the food we eat. With a 2021 US study finding that PFAS was present in plant-based drinking straws, researchers from the University of Antwerp in Belgium analyzed straws made of various materials to see if the same was true in Europe.

The researchers tested 39 different brands of straws made from paper, glass, bamboo, stainless steel, and plastic, and analyzed them for 29 different PFAS compounds.

The majority of brands tested (69%) contained PFAS, with 18 different PFAS detected in total. Paper straws were most likely to contain PFAS, with the chemicals detected in 90% of the brands tested, albeit in highly variable concentrations. Perfluorooctanoic acid (PFOA), a compound linked to high cholesterol, a reduced immune response, thyroid disease and increased kidney and testicular cancer, was most frequently detected. PFOA has been banned globally since 2020. Also detected were trifluoroacetic acid (TFA) and trifluoromethanesulfonic acid (TFMS), ultra-short-chain PFAS that are highly water-soluble and so might leach out of straws into drinks.

Bamboo straws fared only slightly better than paper ones, with PFAS found in 80% of brands tested. The chemicals were found in 75% of plastic straws and 40% of glass brands. PFAS were not detected in any of the steel straws tested.

"Straws made from plant-based materials, such as paper and bamboo, are often advertised as being more sustainable and eco-friendly than those made from plastic," said Thimo Groffen, the study's corresponding author. "However, the presence of PFAS in these straws means that's not necessarily true."

The PFAS concentrations were low and, the researchers say, pose a small risk to human health. However, the problem with PFAS is that they're bioaccumulative, meaning they can build up over time because they're absorbed but not excreted.

"Small amounts of PFAS, while not harmful in themselves, can add to the chemical load already present in the body," said Groffen.

The researchers say that while the study did not determine whether PFAS were added to the straws or were the result of contamination – for example, from the soil in which the plant-based materials are grown – the presence of the chemicals in almost every brand of paper straw means it's

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likely that, in some cases, PFAS were used as a water-repellent coating. The study also did not examine whether PFAS leached out of the straws into the liquid they were sitting in.

To be safe, the researchers suggest people start using stainless steel straws, or ditch straws altogether.

"The presence of PFAS in paper and bamboo straws shows they are not necessarily biodegradable," Groffen said. "We did not detect any PFAS in stainless steel straws, so I would advise consumers to use this type of straw – or just avoid using straws at all."

The study was published in the journal Food Additives and Contaminants.

New Atlas, 24 August 2023

https://newatlas.com

Our plastic waste can be used as raw material for detergents, thanks to an improved catalytic method

2023-08-16

But, for researchers at UC Santa Barbara, one person's single-use packaging is another person's useful raw material. In a paper published in the journal Chem, they have reimagined the value of single-use plastics, with improvements to an innovative process that can turn polyolefins, the most common type of polymer in single-use packaging, into valuable alkylaromatics — molecules that underlie surfactants, the active components of detergents and other useful chemicals.

"If we make these surfactants from fossil fuels now and you could make them from waste plastics, then you are not using fossil fuels to make surfactants anymore, and you're getting another use out of the carbon that went into the plastics," said chemical engineering professor Susannah Scott, who holds UCSB's Mellichamp Chair in Sustainable Catalytic Processing. Instead of burning them or burying them in landfills — practices that represent the major ways we currently deal with plastic waste — plastics are repurposed in a method that shortcuts conventional "dirty" processes for making surfactants while giving single-use plastics one more shot at usefulness.

The researchers built on previous work in which they debuted a catalytic method to break the strong carbon-carbon bonds that make plastic the difficult-to-degrade material it is, then rearrange the molecular chains into alkylaromatic rings. While effective, Scott said, the original process, based

We've managed to accumulate so much plastic trash that it's daunting to think about what could be done with the tons upon tons of nonbio-degradable waste. And as much as we are trying to scale back our dependence on single-use plastics, we continue to add to the global plastic trash hoard. Events like the COVID-19 pandemic only served to expand their use for personal protective equipment and disposable and take-away packaging.

on a platinum-on-alumina catalyst, was slow, and its yield of alkylaromatic molecules was low. "What we've done in this paper is show how to do it much better," she said.

Key to their method is increasing the acidity of the original alumina catalyst, via the addition of chlorine or fluorine. With the added acid sites, the team was able to boost the speed and selectivity of their process.

"It just screams along," Scott said. "It makes the alkylaromatics faster, and we can tune it to make the right-size molecules." In the new paper, they focused on finding the optimal ratio of acid sites to metal sites in their catalyst, she explained. "It turns out they work together. They have different roles, but you need both of them to be there and in the right ratio so the catalytic cycle doesn't get stuck at any point."

In addition, their one-pot process operates at moderate temperatures, requiring a low energy input. While the method originally took 24 hours to turn plastic into alkylaromatic molecules, the improved process can complete the task within a couple of hours, increasing the amount of plastic that can be converted in a reasonably-sized reactor.

"If we make these surfactants from fossil fuels now and you could make them from waste plastics, then you are not using fossil fuels to make surfactants anymore, and you're getting another use of the carbon that went into the plastics."

With further improvements, this method could be on its way to becoming a viable commercial process, according to Scott. The ultimate goal is to bring it into wide use, which would enable and incentivize the recovery of single-use plastics. Using waste plastics as a highly abundant raw material, chemical companies could take the alkylaromatic molecules resulting from this process and transform them into the surfactants that are formulated into soaps, washing liquids, cleansers and other detergents.

"Ideally you want to reuse waste plastic for a purpose with a large enough production volume, for which there is significant demand, in order to make a dent in the plastic problem," Scott explained. To determine if this method is truly sustainable, she added, it would have to undergo a lifecycle assessment, in which the energy spent and greenhouse gasses emitted are calculated at each step. Using waste material ensures that no additional greenhouse gas emissions are produced to create the feedstock, but the energy required to run the catalytic process and separate the desired molecules would have to be factored in before scaling up, Scott said. If it passes muster, the method could displace the

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more fossil fuel-intensive processes that go into creating surfactants from scratch.

"We will need multiple targets to deal with the waste plastic problem, but this is a fairly big one," Scott said. "This is worth doing."

Research on this study was also conducted by Jiakai Sun, Yu-Hsuan Lee and Mahdi M. Abu-Omar at UCSB; Ryan D. Yappert and Baron Peters at University of Illinois, Urbana-Champaign; and Anne M. LaPointe and Geoffrey W. Coates at Cornell University.

us Santa Barbara, 16 August 2023

https://ucsb.edu

Researchers produce polymers from ballbot-type carbenes for the first time

2023-08-28

Using such "ballbot molecules," and working together with Chinese researchers, the Münster physicists and chemists have succeeded for the first time in making the halogenated NHCs produce long-chain mobile polymers—chains of molecules—on metallic surfaces. Details of the work have been published in the journal Nature Chemistry.

The mobility of the ballbot-type NHCs opens up new possibilities, for example self-assembly into highly ordered domains from this type of molecule, up to cooperative, swarm-type behavior on the part of the NHCs in autonomously converting certain metallic surfaces into a different highly-ordered structure without any external influence such as light or electrons.

"Over and above the self-organization, these ballbot polymers hold great promise for new applications in nanoelectronics, surface functionalization and catalysis," says Prof. Harald Fuchs, Senior Professor at Münster University's Institute of Physics and Scientific Director of the Center for NanoTechnology (CeNTech) at Münster.

NHCs can be be easily modified in the nitrogen (N) groups of the five-fold heterocyclic body of the molecules. As a result, this makes it possible not only to influence the electronic interaction between the carbenes and the atoms of a metallic surface—for example, gold—but also to control the alignment of the carbenes vertically or parallel to a surface.

N-heterocyclic carbenes (NHCs) are small, reactive ring molecules that bond well with metallic surfaces, and which over the past few years have attracted a great deal of interest in the field of the stable chemical modification of metallic surfaces. One property—discovered at the University of Münster in Germany a few years ago—is the ability that certain NHC derivatives have, not only to anchor themselves to individual metal atoms, but also to completely extract an individual atom from the surface. Having bonded with these so-called adatoms, the NHCs glide freely over the surface—like a ball-

One special feature of the halogenated NHCs used, which were developed at the Institute of Organic Chemistry at the University of Münster, is their ability to spontaneously form adatoms on noble metals and the mobility which arises as a result. This is a prerequisite for their coming together and for the reaction with other reactive systems on the surface.

"A decisive factor in the success of the experiments was the balance between the chemical reactivity of the monomeric structural units and their mobility," says lead author Prof. Jindong Ren, formerly a postdoctoral researcher in Prof. Harald Fuchs's group and now a principal investigator (PI) and group leader at the National Center for Nanoscience and Technology (NCNST) of China.

On the one hand, the monomers can move easily on the surface due to their ballbot property; on the other hand, the contact time which the parties to the reaction have needs to be of a sufficient length to make the reaction happen. This occurs above all through the molecular structure and a suitable temperature setting during the experiment.

Controlling the chemical reactions and providing evidence for the desired reaction products in the field of precision chemistry for surfaces requires highly specialized preparative and analytical experiments that allow molecular interactions on surfaces and individual reaction steps at a submolecular scale to be observed.

For this purpose, the researchers at CeNTech, NCNST and at Beijing National Center for Condensed Matter Physics and Institute of Physics employed scanning probe microscopy methods (STM and nc-AFM), as well as photoemission spectroscopy, to clarify the chemical bonding taking place and to provide evidence of the ballbot structures.

The experimental results were complemented by elaborate computer simulations at the Institute of Solid State Theory at Münster University, based on quantum mechanics approaches and reactive force fields. In this way, the team confirmed the experimental results and quantified the electronic and structural properties of the ballbot polymers.

Precision chemistry on surfaces has now evolved into a separate area of chemistry. Unlike in traditional chemistry in a test tube or the gas phase, this particular branch of chemistry requires ultra-high vacuum conditions, and often, temperatures as low as minus 268 degrees Celsius in order to avoid any unintentional contamination, as well as to enable the observation of chemical (intermediary) steps at the molecular level.

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Solid surfaces—usually crystalline—serve as the platform (substrate) for the reaction and they can also support the reaction catalytically. Nano-structured surfaces, such as those used in the work described above, make it possible to control not only the alignment, but also a selective geometric arrangement of the reaction products or of the resultant polymers.

Phys Org, 28 August 2023

https://phys.org

Zinc-air battery could be about to take off

2023-08-26

"These have been in the market for years now, but they're not chargeable. They're just one time use," says Dr Muhammad Rizwan Azhar, a researcher at Edith Cowan University (ECU) and co-author on a paper recently published in EcoMat.

But now Azhar and colleagues have developed a rechargeable zinc-air battery – and they have electric vehicles in their sights.

"We have tested it for 950 hours, it doesn't lose any power, it can be continuously charged and discharged," he says.

The difference between this battery and conventional disposable ones is the material in the battery cathode. The team has developed a cathode made from nickel, iron, carbon and a small amount of cobalt.

"The cathode material, which acts as a catalyst, gets oxygen from the air to get charging and discharging happening," says Azhar.

"Once it's been used, it gives back that oxygen."

Batteries work by performing a chemical reaction that releases energy – in rechargeable batteries, it's a reversible reaction.

In the case of a zinc-air battery, that reaction happens between zinc and oxygen – as Azhar says, "it's breathing air".

The battery they've developed can stay stable for a long time, and has a high peak power density, making it very efficient.

"We have tested these batteries for 3-4 years now, in individual cells. We are in the process of scaling it up as a larger cell and also a battery pack in different cells together, and then putting them for a real time application in a in an EV," says Azhar.

Zinc is a very useful battery material, especially when in combination with oxy-gen. Zinc-air batteries can be a powerful and safer alternative to lithium-ion, but until now, they've had one key fault. And it's a big one.

The team hopes to test out the zinc-air battery in ECU's motorsports discipline.

"Our students and staff there make a racing car. We are in the process putting [our battery] into our motorsports car."

Azhar would eventually like to see onshore manufacturing of zinc-air batteries in Australia.

"If we have the interest and enthusiasm from industry and government as well, the research can be very quickly transformed into products," he says.

"Australia has the largest reserves of zinc, which will be used for these types of batteries."

Cosmos, 26 August 2023

https://cosmosmagazine.com

Some Menstrual Products Contain PFAS

2023-08-11

At this year's American Chemical Society fall meeting, researchers from Professor Graham Peaslee's laboratory at the University of Notre Dame present new evidence that some menstrual products contain per- and polyfluoroalkyl substances, or PFAS. Based on the high concentrations of fluorine in some products, the researchers suggest their use is intentional by manufacturers.

Fluorine in menstrual products is an indicator of PFAS

Also known as "forever chemicals", PFAS is an umbrella term that accounts for approximately 12,000 compounds that are stain-, stick- and water-resistant. While these properties might seem useful for consumer products like food packaging or pots and pans, PFAS do not break down very easily. Instead, they bioaccumulate, and have been associated with adverse effects on the environment and human health.

Peaslee's laboratory has analyzed many consumer products for fluorinated compounds, an indicator of potentially harmful PFAS, including school uniforms, cosmetics and food packaging. This is the first time they've turned their attention to menstrual products, an idea put forward by Alyssa Wicks, a graduate student in the lab.

The Peaslee laboratory uses a rapid screening technique called particle-induced gamma-ray emission (PIGE) spectroscopy, which is considered a

Menstrual products – including tampons, panty liners, pads and menstrual cups – are used during a menstrual bleed to help people feel more comfortable and sanitary. Approximately 22 menstrual products are used each cycle, equating to ~11,000 products in a lifetime. Unfortunately, there are menstrual product manufacturers that fail to list the ingredients of their products on the packaging, meaning customers might be unaware of what they are using on or in their bodies.

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gold-standard tool for detecting light elements in depths of surface layers. "Our first step was a screening that's done quickly and simply," says Wicks. "We determined if these products had organic fluorine as a surrogate for PFAS." A total of 123 menstrual products that are sold in the US were analyzed.

Wicks cut small portions of each item and analyzed them using PIGE spectroscopy in under three minutes. For menstrual products that contain multiple layers, such as pads and period underwear, the layers were sampled separately. Wicks also measured total fluorine levels in the packaging of some single-use menstrual products like tampons.

Menstrual underwear has high levels of fluorine

The analyses suggest that, from the products tested, there's a mixed bag in terms of which ones may contain PFAS. "In general, tampons didn't seem to contain fluorine," says Wicks. "Same with menstrual cups and the layers of pads that come in contact with a person's skin." However, the presence of total fluorine in the wrappers for pad and tampon products, and the outer layers of the period underwear products, was much higher – in some instances, 1,000 to several thousand parts per million total fluorine.

Wicks suggests that, for the menstrual underwear products, the levels of fluorine were high enough that the team consider their use in these products to be intentional: "The levels were high enough that we would consider it to contain polymeric PFAS, which when they make the synthetic fibers that are in the underwear, they are adding PFAS to these fibers," she explains. Wicks suggests that PFAS might be utilized in wrappers to prevent moisture from affecting the products, and in the case of menstrual underwear, to prevent leakage of blood from the outer layers of period that might stain clothing.

Should menstrual product users be concerned?

Peaslee emphasizes that, currently, there is no safe PFAS that scientists are aware of. If PFAS are present in menstrual products, it's not only a concern for the wearer but also for the environment. "Luckily, there are thousands of studies published on the ecological and health impacts of PFAS. Very low concentrations correlate with adverse health effects. In humans, they're concerned with several types of cancer, hypertension, ulcerative colitis and even thyroid disease," Peaslee explains. "Of course, you're concerned for the wearer, but we're also concerned about the ecological impact because PFAS are 'forever chemicals'. Once these products are thrown away, they go to landfills and decay, releasing PFAS into

groundwater. And we, or later generations, could end up inadvertently ingesting them."

Next, Wicks plans to run deeper analyses on the products tested, and include samples from other countries outside of the US: "We used PIGE as a way to quantify the total fluorine in our samples. PIGE is a great tool, but it doesn't tell you what specific PFAS compounds are in all of these products," she says. "To figure that out, we need to do targeted analyses using liquid-chromatography with tandem mass spectrometry (LC-MS-MS) where we target for 31 PFAS compounds. We just got our new PFAS compound standard set, so I'll be busy these upcoming weeks doing targeted analyses to look for trends in what types of PFAS are being found in these products," says Wicks.

The scientists believe that the absence of fluorine in some products tested is encouraging, as it implies the use of PFAS is not essential in this context. "Feminine products are essential, but the need for a fluorinated wrapper, or the need for a fluorinated layer, doesn't seem to be, because plenty of them are made without relying on these compounds," Peaslee says.

This article is based on research findings that are yet to be peer-reviewed. Results are therefore regarded as preliminary and should be interpreted as such. Find out about the role of the peer review process in research here. For further information, please contact the cited source.

Technology Networks, 11 August 2023

https://technologynetworks

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Novel chemosensor-based method for rapid detection of bacterial toxin

2023-08-30

This molecule, which is found in the outer membrane of Gram-negative bacteria, can be very harmful to humans. It can trigger a major immune response, producing fever and inflammation. In the worst cases, it can cause organ failure due to sepsis.

Surprisingly, for such a ubiquitously present toxin, there are very few ways to effectively detect the presence of LPS. The gold standard for its detection is the limulus amebocyte lysate (LAL) test. Because this has to be done manually in a clean laboratory setting, the procedure can take several hours and is also expensive.

While there are other methods to detect LPS, they too are time-consuming or cumbersome. And the time taken here can sometimes cause significant delays in decision-making at hospitals and pharmaceutical manufacturing sites.

Against this backdrop, a research team from Japan have pioneered a new strategy to quickly detect LPS in soluble samples. In their latest study, published in the journal Analytical Chemistry, the team presents a promising platform that could revolutionize how we screen for LPS.

The first author of the study is Hiroshi Kimoto, who is a Ph.D. student at Sophia University, Japan, and a member of the Technical Development Division at Nomura Micro Science Co., Ltd. The study was co-authored by Takashi Hayashita and Takeshi Hashimoto, both from Sophia University, and Yota Suzuki from Saitama University.

The main component of the proposed LPS analysis system is a ratiometric fluorescent chemosensor called Zn-dpa-C2OPy. This compound, which was designed to bind selectively to LPS, exhibits interesting fluorescent properties. When not bound to LPS, it forms small spherical vesicles that emit light with a certain wavelength when excited by UV rays.

However, in the presence of LPS, the chemosensor forms complex aggregates with the toxin in a solution; these aggregates are structurally distinct from the aggregates of either the chemosensor or LPS alone. The complex chemosensor-LPS aggregates emit light at a completely different wavelength when excited by UV rays, and their presence was further verified via spectrometric measurements.

The COVID-19 pandemic made it very clear that we need better methods to quickly screen for dangerous pathogens and substances. One such compound that regularly flies under the radar is lipopolysaccharide (LPS), largely known as "endotoxins."

To achieve high-throughput LPS detection, the researchers combined the chemosensor with a flow injection analysis (FIA) system and a self-developed dual-wavelength fluorophotometer. This system allows one to easily mix a liquid sample of interest with a known quantity of chemosensor, and the mixture is then fed into the fluorophotometer, which measures the fluorescence changes in response to LPS. Based on the ratio between the fluorescence intensities, one can estimate the concentration of LPS in the input sample.

One of the main benefits of this system is its speed. "It takes only one minute from sample collection to analysis results, with an hourly sample throughput of 36, making this technique extremely rapid and efficient," says Kimoto.

In addition to the high throughput, the proposed chemosensor exhibits high sensitivity and stability to quantify LPS. In fact, the chemosensor has a detection limit of 11 pM (picomolar), which is lower than that of other reported small molecule chemosensors for LPS detection. This means that it can detect lower concentrations of LPS than other alternative methods can.

Moreover, the chemosensor-based analysis system is simple and animal-friendly—other conventional LPS detection methods use animal resources and may, in turn, harm these animals. This makes it a great candidate for practical and efficient point-of care testing for LPS and bacterial contaminations in water, clinical, or pharmaceutical samples.

Envisioning the long-term implications of this work, Mr. Kimoto comments, "Based on this research, an online-endotoxin monitor will be developed and made available for use in real-life situations. Such a monitor could be installed at pharmaceutical production sites, hospital bedsides, and intensive care units to continuously monitor endotoxin concentration in pharmaceutical products, such as water for injection, or the blood of infected patients."

With more work in the field, the threat of endotoxins will be minimized in the near future, making hospitals safer and improving diagnostic procedures for bacterial diseases.

Phys Org, 30 August 2023

https://phys.org

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Titanium spikes kill superbugs drug-free by literally ripping them apart

2023-08-30

Surgery can lead to infection, and, with the rise in drug-resistant microbes, providing effective treatment is becoming mor difficult. While bacteria are usually the main infection-causing culprits, drug-resistant species of Candida, a type of fungus, are also proving problematic. Not only can they effectively colonize and form biofilms on implanted materials, leading to hospital-acquired infections, but they also lead to poor clinical outcomes.

When they're inserting things like titanium hips or dental prostheses, doctors use a range of antimicrobial coatings, chemicals and antibiotics to prevent infection from developing. But these measures won't be as effective, or effective at all, if the microbe in question has developed resistance.

But, researchers from RMIT University have come up with a novel, drug-free way to kill superbugs that's inspired by the antimicrobial surface on the wings of some insects. Insects such as dragonflies, cicadas, and damselflies have tiny pillars – nanopillars – on the surface of their wings that act as a "mechano-biocidal," physically pulling apart bacterial cells and killing them.

"It's like stretching a latex glove," said Elena Ivanova, corresponding author of the study. "As it slowly stretches, the weakest point in the latex will become thinner and eventually tear."

So, the researchers set about creating their own mechano-biocidal, developing a titanium surface covered with specially designed microscale spikes, each about the size of a bacteria cell, using a technique called plasma etching.

They tested the effectiveness of the surface in killing multi-drug-resistant Candida and found that about half the cells were destroyed soon after making contact with the spikes. Significantly, the other half – the cells that were not immediately destroyed – were injured enough that they were unable to reproduce or cause infection.

"The Candida cells that were injured underwent extensive metabolic stress, preventing the process where they reproduce to create a deadly fungal biofilm, even after seven days," said Denver Linklater, one of the study's co-authors. "They were unable to be revived in a non-stress

Inspired by the bacteria-killing structures seen on the wings of some insects, researchers have developed a drug-free way to kill off drug-resistant microbes that commonly cause hospital-acquired infections. Their technique is a novel and effective way of tackling the problem of antibiotic-resistant superbugs.

environment and eventually shut down in a process known as apoptosis, or programmed cell death."

The micropillared titanium surface had already been found to be effective against two common pathogens, Staphylococcus aureus ('Golden Staph') and Pseudomonas aeruginosa bacteria, in a previous study published in the journal Materialia.

"The fact that cells died after initial contact with the surface – some by being ruptured and others by programmed cell death soon after – suggests that resistance to these surfaces will not be developed," Ivanovna said. "This is a significant finding and also suggests that the way we measure the effectiveness of antimicrobial surfaces may need to be rethought."

The researchers say the relatively simple plasma etching technique they used to create the spikes could be applied across a wide range of materials and applications.

"This new surface modification technique could have potential applications in medical devices but could also be easily tweaked for dental applications or for other materials like stainless steel benches used in food preparation and agriculture," said Ivanovna.

The study was published in the journal Advanced Materials Interfaces.

New Atlas, 30 August 2023

https://newatlas.com

Cancer drug kills 'silent' HIV in cell and mice study

2023-08-31

A new mouse study has discovered that an existing cancer drug can kill some 'silent' HIV infected cells. The researchers are excited about their finding and are moving into clinical trials in humans.

However, questions remain about whether this could be a 'cure', or just a way to limit the number of these cells in the body. The research has been published in Cell Reports Medicine.

"Currently, for people living with HIV, they have to take antiretroviral medication their whole life. As soon as they've stopped taking antiretroviral medication, the virus rebounds," one of the researchers, Dr Philip Arandjelovic told Cosmos.

The research was led by Arandjelovic at WEHI, the Walter and Eliza Hall Institute of Medical Research, in Melbourne and Youry Kim from the Doherty Institute.

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"What we found was that using a preclinical mouse model of HIV infection, we could use a preexisting, repurposed anti-cancer drug called venetoclax to delay how long it takes the virus to reemerge in the body after we stop standard treatment," Arandjelovic told Cosmos.

HIV (human immunodeficiency virus) is a virus which can infect humans, and over time causes the immune system to slowly fail.

Although current HIV medication – called antiretroviral therapy (ART) is effective at killing the HIV that is damaging the body and immune system, it can't kill every single viral particle as some HIV hides or hibernates inside our cells. This is similar to malaria and chickenpox (or shingles as it's known when it reappears). This "silent" HIV emerges from the cells when ART is stopped and begins to 'repopulate' the lost HIV in the body, again causing symptoms.

The team looked at the cancer drug venetoclax, as well as another potential cancer drug which is currently going through clinical trials called S63845, to see if they could attack the silent HIV while still in the cell. This could potentially remove the reservoir of virus.

Specifically, both the venetoclax and S63845 targets cells that are using more 'pro-survival' proteins. This means that some normal cells also die, but mostly it targets the HIV cells.

"Venetoclax specifically targets those pro-survival proteins and inhibits them," says Arandjelovic. "It does that in cancer cells, but it can also do it in any other cell that's addicted to these pro-survival proteins."

The researchers at the Doherty Institute used cells from humans currently with HIV on ART, and the team at WEHI looked at mice which have been genetically engineered to be immunology similar humans. These are called "hu-mice" and were also infected with HIV and put on ART therapy.

In the cell part of the study, both venetoclax and S63845 were effective at killing the HIV virus and the cells that were harbouring them.

The WEHI team found that in the hu-mice, venetoclax delayed the time to viral rebound compared to a control by a week, while the 2-drug combination delayed the viral rebound an extra week on top of that.

Unfortunately, even when venetoclax and S63845 were used together, it couldn't completely destroy all of the HIV cells in the hu-mice. The team could tell that it was working because it took those mice longer to 'rebound' back to higher HIV levels.

This is a good start, but it's not a cure currently. Even if only a fraction of HIV cells remain, it could be enough to re-establish a population of HIV in the body. This was the case in the mice.

However, the team is moving towards clinical trials as they believe that humans might respond better than mice when it comes to 'finishing off' the last few cells.

"While our humanised mouse model is really sophisticated in a lot of ways … it doesn't predict a full human response," Arandjelovic told Cosmos.

The hu-mice "do have these immune cells, they don't function exactly as a healthy humans' immune system does. They don't mount the strong anti-HIV response that typically we get in humans."

Human trials with venetoclax should provide more information about whether a human immune response can limit the HIV that rebounds. The team are currently not pursuing a trial with both drugs simultaneously because S63845 is not available on the market.

Other researchers who weren't involved in the research have also commented on the paper.

"The paper from Arandjelovic, Kim and co-authors shows that approaches previously used for the successful treatment of certain types of blood cancers increase the time to viral rebound in a humanised mouse model of HIV infection following anti-retroviral treatment interruption," says Professor Anthony Kelleher, a Director of the Kirby Institute which investigates infectious diseases, including HIV.

"While the effect is present using one drug, currently in routine clinical use, the effect is best observed using the first drug in combination with a second drug, which is in early phase development."

Cosmos, 31 August 2023

https://cosmosmagazine.com

Adapting Ritalin to tackle cocaine abuse

2023-08-30

According to the Centers for Disease Control and Prevention, more than 5 million Americans reported actively using cocaine in 2020, and almost 25,000 Americans died of a cocaine-related overdose in 2021. Although small-molecule drugs have proven effective in treating other drug addictions—for example, methadone as a therapy for heroin abuse—no such medication exists for cocaine abuse.

Cocaine use continues to be a public health problem, yet despite concerted efforts, no drugs have been approved to resolve cocaine addiction. Research suggests that the attention-deficit/hyperactivity disorder drug methylphenidate (MPH; Ritalin) could serve as a cocaine-replacement therapy, but clinical results have been mixed. Although several labs have produced MPH derivatives for testing, parts of the molecule remained chemically inaccessible. Now, researchers reporting in ACS Central Science have cleared that hurdle.

MPH has been considered a potential treatment because it behaves similarly to the illicit drug, increasing dopamine levels in the brain by blocking dopamine reuptake. Additionally, clinical studies have shown that MPH has a lower risk of abuse than cocaine.

Although studies in animals have shown that MPH can reduce cocaine dependence, studies in humans have offered more mixed results. Thus, researchers are developing libraries of MPH derivatives, searching for molecules with improved clinical efficacy. Until recently, however, it was difficult to create derivatives of one chemical component of MPH: its piperidine ring. W. Dean Harman and colleagues wanted to address this shortcoming by taking an organometallic approach.

Using a tungsten-based reagent, the researchers synthesized a library of MPH analogs specifically modified at the piperidine ring with a variety of chemical groups. And whereas MPH is a mixture of four isomers—otherwise identical molecules with small structural differences—the new method allowed the researchers to synthesize and purify compounds that were predominantly comprised of a single isomer.

This could be important in clinical studies, as different isomers of some drugs can have significant impacts on therapeutic efficacy or safety. Whether any of these MPH analogs prove effective against cocaine addiction remains to be determined, but the researchers noted that the new protocol could be widely applicable to pharmaceutical development, given the ubiquity of the piperidine ring in small-molecule drugs.

Phys Org, 30 August 2023

https://phys.org

Chemical Mixture Composition Determined Rapidly Using Nothing But Images

2023-08-30

Have you ever accidentally ruined a recipe in the kitchen by adding salt instead of sugar? Due to their similar appearance, it's an easy mistake to make. Similarly, checking with the naked eye is also used in chemistry labs to provide quick, initial assessments of reactions; however, just like in the kitchen, the human eye has its limitations and can be unreliable.

Machine learning model provides quick method for determining the composition of solid chemical mixtures.

To address this, researchers at the Institute of Chemical Reaction Design and Discovery (WPI-ICReDD), Hokkaido University led by Professor Yasuhide Inokuma have developed a machine learning model that can distinguish the composition ratio of solid mixtures of chemical compounds using only photographs of the samples.

The model was designed and developed using mixtures of sugar and salt as a test case. The team employed a combination of random cropping, flipping and rotating of the original photographs in order to create a larger number of sub images for training and testing. This enabled the model to be developed using only 300 original images for training. The trained model was roughly twice as accurate as the naked eye of even the most expert member of the team.

"I think it's fascinating that with machine learning we have been able to reproduce and even exceed the accuracy of the eyes of experienced chemists," commented Inokuma. "This tool should be able to help new chemists achieve an experienced eye more quickly."

After the successful test case, researchers applied this model to the evaluation of different chemical mixtures. The model successfully distinguished different polymorphs and enantiomers, both of which are extremely similar versions of the same molecule with subtle differences in atomic or molecular arrangement. Distinguishing these subtle differences is important in the pharmaceutical industry and normally requires a more time-consuming process.

The model was even able to handle more complex mixtures, accurately assessing the percentage of a target molecule in a four-component mixture. Reaction yield was also analyzed, determining the progress of a thermal decarboxylation reaction.

The team further demonstrated the versatility of their model, showing that it could accurately analyze images taken with a mobile phone, after supplemental training was performed. The researchers anticipate a wide variety of applications, both in the research lab and in industry.

"We see this as being applicable in situations where constant, rapid evaluation is required, such as monitoring reactions at a chemical plant or as an analysis step in an automated process using a synthesis robot," explained Specially Appointed Assistant Professor Yuki Ide. "Additionally, this could act as an observation tool for those who have impaired vision."

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Reference: Ide Y, Shirakura H, Sano T, et al. Machine learning-based analysis of molar and enantiomeric ratios and reaction yields using images of solid mixtures. Ind Eng Chem Res. 2023:acs.iecr.3c01882. doi: 10.1021/acs.iecr.3c01882

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Technology Networks, 30 August 2023

https://technologynetworks.com

Novel recycling process gives old plastics new life: Researchers break down, rebuild polyurethane to make new foam

2023-08-29

Polyurethane plastics are ubiquitous, used everywhere from mattresses to shoes. But once these products are no longer wanted, these materials litter landfills and oceans across the world.

Now, a group of researchers at Northwestern University has developed a new recycling method for polyurethane foams, one of the most common types of plastic, that uses nontoxic, greener catalysts, as described in a paper published Aug. 27 in the journal Macromolecules.

The process involves chemical reactions that simultaneously reprocess and "refoam" polyurethane after heating in the presence of a zirconium-based catalyst and foaming agent is introduced. The recycled foam maintained its durability and structural and chemical integrity. The process is described in a related paper published earlier this month in the journal Advanced Materials.

William Dichtel, the Robert L. Letsinger Professor of Chemistry at Northwestern's Weinberg College of Arts and Sciences, led the research team and called the breakthrough finding a "major step forward." When plastics with a circular life cycle are produced, they become an important part of the economy of the future.

"The types of polymers that require this catalyst approach are called thermosets, or crosslinked polymers," said Dichtel, who is a faculty affiliate at Northwestern's Paula M. Trienens Institute for Sustainability and Energy. "Thermosets are important because of their superior durability and stability, but these properties come at the expense of recyclability. New methods to recycle thermosets will reduce greenhouse emissions, save energy and decrease landfill use."

This "circular life cycle" refers to materials that are reprocessed or remanufactured with minimal loss of quality and value, rather than being used once and discarded or destroyed.

Traditional polymer plastic recycling involves melting down the plastic and then casting it for a new use. But more durable plastics—like polyurethanes from spray-foam insulation, car interiors and types of apparel—don't melt down because of their crosslinked structure.

Dichtel and his team developed a method to recycle and reshape existing polyurethane foam products by incorporating a zirconium-based catalyst into the material after it is blended into smaller pieces using a kitchen blender. They had previously relied on tin-based catalysts for this process, but these catalysts are too toxic to be explored further.

When the polyurethane is heated, the zirconium catalyst rearranges its bonds and allows the material to be reshaped. At the same time, a substance called a foaming agent generates new gas bubbles, which are trapped within the plastic. In this way, the old polyurethane foam, typically only used once, is transformed into a new, reshaped foam.

The discovery builds on Dichtel's prior research that established a way to recycle polyurethane foam into solid plastics. These results were an important step toward polyurethane circularity; however, solid plastic products produced in the study are not used commercially. The ability to recycle one foam into another foam product projects to be far more important and was enabled by a key collaboration with scientists from BASF, a major polyurethane producer.

Implications of the new technique are global, according to the study. The discovery could be applied to post-consumer polyurethane foam products or unused industrial scrap plastics.

"We are excited to work with our partners at BASF, one of the most important and innovative polyurethane producers in the world, to continue our quest to make polyurethane more circular and sustainable," Dichtel said of the next steps.

Phys Org, 29 August 2023

https://phys.org

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World-first drug lowers genetic form of "bad cholesterol" by up to 65%

2023-08-29

Studies have shown that high levels of lipoprotein(a) or Lp(a), pronounced "L-P-little-A", increase the likelihood of heart attack or stroke, particularly with familial hypercholesterolemia, an inherited condition characterized by high cholesterol. Lp(a) is a type of low-density lipoprotein (LDL) cholesterol, otherwise known as 'bad cholesterol,' but it's stickier, increasing the risk of blockages and blood clots (atherosclerosis) forming in the arteries.

Commonly used cholesterol-lowering drugs such as statins don't have the same effect on Lp(a), and because it's largely caused by genetics, Lp(a) is also difficult to control through diet, exercise and other lifestyle changes. There are no approved medications currently available that target Lp(a).

However, a team led by researchers at Monash University have developed and tested a groundbreaking, world-first oral medication, muvalaplin, that interrupts the body's ability to form Lp(a).

"When it comes to treating high Lp(a), a known risk factor for cardiovascular disease, our clinicians currently have no effective tools in their kit," says Stephen Nicholls, the study's lead author. "Lp(a) is essentially a silent killer with no available treatment, this drug changes that."

Lp(a) is composed of one molecule of an LDL-particle containing apolipoprotein B100 (apo B100) and one molecule of a glycoprotein called apolipoprotein(a), or apo(a). Mulvalaplin disrupts the interaction between apoB100 and apo(a), resulting in lower Lp(a) levels.

The trial enrolled a total of 114 participants; 89 were treated with muvalaplin, and 25 were given a placebo. The trial was conducted in two parts. The first part evaluated the effect of only one dose of muvalaplin in ascending increments, from 1 mg to 800 mg, in healthy participants with a mean age of 29. The second part evaluated the effect of a single daily dose in ascending increments (30 mg to 800 mg) taken over 14 days by healthy participants whose mean age was 32 and who had elevated Lp(a) plasma levels.

Baseline Lp(a) and LDL cholesterol levels were taken at the start of the trial and the effect of muvalaplin on Lp(a) levels observed. The researchers saw reduction in Lp(a) levels from baseline as early as day two with the

Researchers have developed the world's first oral drug to target a form of cholesterol that has previously been untreatable and is largely caused by genetics, making it difficult to control by way of exercise, diet or other lifestyle factors.

participants receiving multiple doses. The reduction in Lp(a) was 64% to 65% at doses of 100 mg or more, occurring on days 14 and 15.

Of participants in the single ascending dose group, the most common adverse events were headache (33%), back pain (13%) and fatigue (11%). The multiple ascending dose group reported experiencing headache (31%), diarrhea (20%), abdominal pain (15%), nausea (10%) and fatigue (10%). No deaths or serious adverse events were reported.

The researchers note the study's limitations, namely that it was a small, phase 1 study. Larger, longer clinical trials in more diverse populations, including those with established cardiovascular disease, will be needed to establish the safety profile of muvalaplin. Additionally, study participants had low-to-moderate elevation of Lp(a) levels; the drug's target audience would likely include people with greater Lp(a) elevations.

Nonetheless, as the first oral agent specifically developed to lower Lp(a) levels, muvalaplin is a promising development.

"This drug is a game-changer in more ways than one," Nicholls said. "Not only do we have an option for lowering an elusive form of cholesterol, but being able to deliver it in an oral tablet means it will be more accessible for patients."

The study was published in the journal JAMA Network.

New Atlas, 29 August 2023

https://newatlas.com

How human recreation alters river chemistry

2023-08-24

Human activities like tubing and swimming significantly impact river chemistry, according to preliminary results from researchers at Johns Hopkins University and Colorado School of Mines that were presented at the autumn meeting of the American Chemical Society (ACS) held in San Francisco, California and virtually.

Last year, the Hopkins-led team examined samples from Clear Creek in Colorado over the busy Labor Day weekend in September – when there can be up to 500 people every hour swimming and tubing in the stream – and again on a quieter weekday afterward. To provide a comparison, they analysed samples taken upstream from an undisturbed spot along the waterway.

Specifically, they were looking for inorganic contaminants, including metals and nanoparticles, as well as organic contaminants like pharmaceuticals. The team also investigated the stream's microbiome.

The analysis turned up illegal drugs like cocaine, the local anaesthetic lidocaine, seizure medications, and plasticisers like phthalates. Organic

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sunscreens and UV filters were also detected, along with the antihistamine fexofenadine, and polyethylene glycol, which is considered a laxative and is also used as a lubricating coating for various surfaces.

All these compounds presumably washed off the skin of people in the creek, or were released in their sweat or urine, among other possible sources, the researchers said.

Noor Hamdan, an environmental engineering PhD student at Hopkins who presented the work at the ACS briefing, explained that the team used liquid chromatography–high resolution mass spectrometry to separate and identify the compounds. 'What we can do with this instrument is blow these compounds into tinier fragments to elucidate their structure and chemical properties, and then we can find out what really is in these samples,' she explained. 'We found that, specifically in the microbial analysis, that the biome composition changes as a function of human recreational activity in the creek.'

Heavy recreation days resulted in elevated major and trace metals, including lead and zinc, Hamdan added, suggesting that humans contribute significantly to resuspending metals and sediment.

Organic sunscreen ingredients like avobenzone and oxybenzone, which have been shown to harm the environment and negative impact aquatic organisms, were also detected.

The researchers searched for the compounds they had found in the US Environmental Protection Agency's Computational Toxicology Chemicals Dashboard (CompTox), which provides public access to chemistry, toxicity, and exposure data.

'What we found is that for a large majority of these compounds, we don't have data on their chronic aquatic toxicity,' Hamdan stated. 'We don't have data on their persistence and their mobility in the environment,' she continued. However, the researchers note that that most of the compounds have low bioaccumulative potential, which means that they won't build up in the bodies of organisms over time.

The team plans to sample Clear Creek again later this year, over Labor Day weekend, and conduct more statistical analysis to confirm that humans really are significantly impacting the stream. Ultimately, they want to collect more samples to track trends over time.

'Most of these compounds that are introduced into the stream are the result of washing off of the body, like sunscreen and personal care

products like fragrances,' said Hamdan. 'If you urinate in the river or you sweat in the river, all of those xenobiotic metabolites can also get into the water.' She also recommends wearing mineral sunscreens, which have ingredients like zinc and titanium and aluminum, and do not contain organic contaminants that can be toxic to aquatic organisms.

However, Michael Focazio, who retired earlier this year from the US Geological Survey where he coordinated the agency's environmental health programme tells Chemistry World that further work is needed to fully understand the study's implications. 'It makes sense that people will be direct sources of these contaminants via swimming and tubing as well as indirect sources as bed sediment is disturbed,' he says. 'But as far as I can tell … there is no perspective provided on other risk sources such as wastewater treatment plant effluents, flooding, etc., which would be needed in order to understand the significance of swimming and tubing.'

Chemistry World, 24 August 2023

https://chemistryworld.com

Phytosterol Supplement Reduces Hearing Loss in Mice

2023-08-25

A new study in mice has shown that phytosterol, a common dietary supplement, may help to reduce age-related hearing loss. The research is published in PLOS Biology.

Cholesterol as part of hearing function

Age-related hearing loss is incredibly common, affecting a third of adults over the age of 65. It is associated with an increased risk of cognitive decline and dementia, so can have important health implications.

Hearing loss with age is thought to be caused by loss of connections between inner hair cells (IHCs) in the inner ear that detect sound and fibers in the auditory nerve, or loss of outer hair cells (OHCs) in a region of the inner ear.

Cholesterol is key to the function of these hair cells, helping them to stretch in response to sound. It has been shown that levels of cholesterol in some areas of the brain can decrease with age, leading the researchers in the current study to investigate if hearing loss could also be related to reduced cholesterol in OHCs.

Phytosterol supplements in models of hearing loss

Aging can trigger cholesterol loss from sensory cells found in the inner ear, linked to hearing loss.

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The researchers analyzed the ears of both young and aged mice, measuring cholesterol content and levels of the enzyme CYP46A1, which helps to break down and recycle cholesterol. Aged mice had more CYP46A1 and less cholesterol in their inner ears than the youngsters.

Next, they over-activated CYP46A1 in the young mice using efavirenz, a drug used to treat HIV/AIDS patients that is also known to activate CYP46A1. Treatment with the drug affected the output of the young mice's inner ears and induced hearing loss, confirming its cause and effect.

But could increasing cholesterol in the brain counter this effect? The researchers gave the mice plant-based cholesterols, called phytosterols, as these can travel through the blood–brain barrier, whereas "normal" circulating cholesterol cannot.

They found that young mice that received both the CYP46A1-activating drug and three weeks of phytosterol supplementation in their diet had improved OHC function.

Further studies needed to confirm

Overall, the findings suggest that aging triggers cholesterol loss from sensory cells found in the inner ear, which can be partly reversed by supplementation with phytosterols. "Altogether, our findings point towards the importance of cholesterol homeostasis in the inner ear as an innovative therapeutic strategy in preventing and/or delaying hearing loss," the authors write in the paper.

As phytosterols can be found in many over-the-counter supplements, the authors note that they could be a convenient way to combat age-related hearing loss. However, further testing in older mouse models as well as in humans will be necessary before more confident conclusions can be drawn.

Reference: Sodero AO, Castagna VC, Elorza SD, et al. Phytosterols reverse antiretroviral-induced hearing loss, with potential implications for cochlear aging. PLOS Biology. 2023;21(8):e3002257. doi: 10.1371/journal.pbio.3002257

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Technology Networks, 25 August 2023

https://technologynetworks.com

Research team clarifies mode of action of cannabinoids in inflammation

2023-08-28

A few days ago, the federal government took the controversial decision to make the acquisition and possession of small amounts of cannabis exempt from punishment. Provided the German parliament approves the draft bill, the "Cannabis Act" will come into force next year. While some consider this move to be long overdue, others continue to warn strongly against the health risks of cannabis use.

The Jena researchers and their colleagues are now taking a different look at cannabis—at the traditional medicinal plant—with a study published in the journal Cell Chemical Biology. The team from the Institute of Pharmacy investigated how certain ingredients from the cannabis plant counteract inflammation. It was already known from previous studies that cannabis is not only an analgesic and an antispasmodic, but also has an anti-inflammatory effect.

"However, the reason for the anti-inflammatory effect was largely unclear until now," says Dr. Paul Mike Jordan, who led the study together with Prof. Oliver Werz.

The researchers studied how different cannabinoids, including the psychoactive THC (tetrahydrocannabinol) and CBD (cannabidiol), which is already found in freely available products today, act on human immune cells. "We found that all eight cannabinoids we studied had anti-inflammatory effects," says Lukas Peltner, doctoral student and first author of the study. "All the compounds we studied were found to inhibit the formation of pro-inflammatory messenger substances in cells while enhancing the formation of inflammation-resolving substances."

CBD induces a switch in immune cells

CBD in particular proved to be highly effective and the team investigated it in more detail with regard to its mode of action. The researchers were able to determine that CBD activates the 15-lipoxygenase-1 enzyme, which triggers the production of inflammation-resolving messenger substances that subsequently cause the inflammation to subside.

"CBD thus induces a switch in the affected cells, so to speak, which steers the inflammatory process from the promoting to the inhibiting side," explains Dr. Jordan. The researchers were also able to confirm these results, which were obtained in cell cultures, in animal experiments on mice.

While the German government is planning to relax legislation on the use of cannabis, researchers from the Friedrich Schiller University Jena, together with colleagues from Italy, Austria and the U.S., have identified the mode of action underlying anti-inflammatory effects demonstrated by cannabinoids.

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In the long term, the insights gained could lead to new therapeutic strategies for treating inflammatory diseases, the researchers conclude. The focus should be on CBD, which was the most effective cannabinoid in the study. Previously approved preparations with cannabinoids contain CBD, "but also the psychoactive THC, which can be associated with a variety of side effects," notes Dr. Jordan. Therapeutics containing only CBD would reduce this problem.

Phys Org, 29 August 2023

https://phys.org

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