CHEMWATCH

Bulletin Board

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ASIA PACIFIC

Rescheduling of bromoxynil products

2024-02-2024

The Australian Pesticides and Veterinary Medicines Authority (APVMA) will take regulatory action on all products containing more than 1.5% weight/volume (w/v) of bromoxynil from 1 June 2024.

This follows a scheduling decision made by the Therapeutic Goods Administration (TGA), the regulatory agency responsible for poison scheduling, to reclassify these products from a Schedule 6 'Poison' to a Schedule 7 'Dangerous Poison'.

The reasoning behind this scheduling decision is published on the TGA website – Notice of interim decisions to amend (or not amend) the current Poisons Standard publication.

Schedule 7 poisons are defined as substances with a high potential for causing harm at low exposure and which require special precautions during manufacture, handling or use. These poisons should be available only to specialised or authorised users who have the skills necessary to handle them safely, including agricultural workers and those with training in pest control. Special regulations restricting the availability, possession, storage or use of Schedule 7 poisons may apply.

Products designated as Schedule 7 poisons are not suitable for use in domestic or home garden situations. Possession, use or supply for domestic or domestic garden purposes is prohibited under the TGA Poisons Standard.

The use of bromoxynil products in accordance with the APVMA-approved label directions is still considered to be safe. However, as a result of the rescheduling of these products to Schedule 7, there will be changes to the signal heading on product labels. These implications will impact those who can access or hold bromoxynil products, and how the product is stored.

The APVMA will work with holders of affected product registrations to make the changes required.

Enquiries about these changes can be directed to enquiries@apvma.gov.au or +61 2 6770 2300.

Media enquiries must be directed to media@apvma.gov.au.

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URL: https://www.apvma.gov.au/news-and-publications/news/rescheduling-bromoxynil-products

Content last updated: 13 February 2024

Content last reviewed: 13 February 2024

Read More

APVMA, 13-02-24

https://www.apvma.gov.au/news-and-publications/news/rescheduling-bromoxynil-products

Proposed changes to the List of chemicals with high hazards for categorisation & information on minor changes to the Guidelines

2024-02-15

In September 2023, we consulted on proposed changes to the Industrial Chemicals (General) Rules 2019 and Industrial Chemicals Categorisation Guidelines (the Guidelines), which included proposals to refine the List of chemicals with high hazards for categorisation (the List).

In this consultation, we provide further details about proposed changes to the List. For example:

- updating the chemicals that are on the List
- a change related to checking esters and salts of chemicals that are on the List – we're seeking your feedback about the chemicals that we will specify and the details of some exceptions that would apply.

We're also providing details of some other minor changes that we'll be making to the Guidelines.

Open for comment until 22 February 2024.

Read More

AICIS, 15-02-24

https://www.industrialchemicals.gov.au/proposed-changes-list-chemicals-high-hazards-categorisation-information-minor-changes-guidelines

AMERICA

How The United States Struggles with Unregulated Toxic Chemicals

2024-02-13

The silent threat of unregulated toxic chemicals in the U.S. is a pressing concern. Unlike strictly regulated pharmaceuticals, these hazardous substances in industrial and commercial products often bypass essential safety checks before entering the market. This detailed exploration sheds light on the consequences, regulatory challenges, and the path toward a healthier, safer future.

Understanding Toxic Chemicals

Toxic chemicals, posing significant risks to human health and the environment, have historically evaded stringent control in the U.S. The 1976 Toxic Substances Control Act (TSCA) left a gap in safety, regulating less than 2% of all manufactured chemicals. Well-known dangers like asbestos and methylene chloride slipped through this regulatory net, exposing the public to untold risks.

2016 Frank Lautenberg Amendments

A pivotal moment in chemical regulation came with the 2016 TSCA amendments, providing the Environmental Protection Agency (EPA) with broader powers. These changes were not just bureaucratic shifts but represented a commitment to safeguarding public health, particularly for vulnerable populations such as children and pregnant women. The amendments symbolized a long-awaited step towards more rigorous oversight of chemical safety.

Read More

One Green Planet, 13-02-24

https://www.onegreenplanet.org/environment/how-the-united-states-struggles-with-unregulated-toxic-chemicals/

Critics: Bill cutting protections from PFAS toxic chemicals a step backward for Indiana

2024-02-12

The definition of PFAS, per- and polyfluoroalkyl substances commonly called "forever chemicals," widely accepted: They are toxic chemicals that

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are dangerous to human health, accumulate in nature and people's bodies, and take thousands of years to break down.

Despite that near universal acknowledgment, Hoosier lawmakers are advancing a bill to change the definition of PFAS — but only in Indiana. In other words, chemicals deemed harmful in every other state will no longer be considered dangerous in Indiana.

In fact, Indiana — already one of the country's most polluted states, according to federal EPA data — wouldn't even recognize those materials as PFAS.

"This bill makes no sense at all," said Gretchen Salter, a strategic advisor for Safer States, a national alliance of environmental health organizations working to provide for a healthier world. "I don't know why anyone would want to limit a state's authority to regulate chemicals that the world has recognized are toxic and harmful to the public."

Proponents of House Bill 1399, including the chemical manufacturing industry, say the change is needed to preserve essential uses of PFAS in items such as medical devices or semiconductors. No one in Indiana, however, is proposing to prohibit those uses.

Read More

Indy Star, 12-02-24

https://www.indystar.com/story/news/environment/2024/02/12/pfas-toxic-forever-chemicals-danger-well-known-but-indiana-lawmakers-try-to-cover-up/72273986007/

Maryland proposes stringent baby food safety regulations

2024-02-12

In a move to safeguard infants from toxic heavy metals, Maryland lawmakers are considering "Rudy's Law," a bill demanding more rigorous testing standards for baby food than those of the U.S. Food and Drug Administration.

In short:

- "Rudy's Law" is inspired by a toddler's lead poisoning from contaminated baby food.

- The bill mandates monthly testing for toxic metals in baby food and requires manufacturers to disclose test results.
- Maryland joins a growing list of states taking action on baby food safety amid slow federal progress.

Key quote:

"There is no safe level of exposure to heavy metals for children and thus, we must do everything that we can to protect this vulnerable age group."

— Sarah Durrin, pediatrician at Children's National Hospital.

Why this matters:

This proposed legislation addresses the importance of proactive measures in food safety, especially for the youngest and most vulnerable. Lead poisoning especially, is an often-overlooked global health crisis.

Read More

EHN, 12-02-24

https://www.ehn.org/maryland-proposes-stringent-baby-food-safety-regulations-2667257365.html

Idaho lawmakers introduce bill to curb pesticide lawsuits, citing exploitation of the legal system by anti-chemical activists

2024-02-24

State senators in Idaho have introduced new legislation that aims to limit chemical exposure and injury lawsuits filed against pesticide manufacturers.

The proposed Senate Bill 1245 would effectively block most failure to warn lawsuits involving pesticides, indicating that any product approved by the U.S. Environmental Protection Agency (EPA), and carrying the agency's required warning label, would have adequate warnings under Idaho state law, regardless of whether there is new evidence that the manufacturers withheld information about known health risks.

The bill has been supported by officials from Bayer, which owns the pesticide Roundup through its Monsanto subsidiary, and testified in support of the bill during an Idaho Senate Commerce and Human Resources Committee hearing on [February 13].

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If the Idaho bill is passed into law, it would effectively block most pesticide lawsuits in that state, according to observers. Some Idaho farming lobbying groups, fearing pesticide restrictions, have also testified in favor of the bill.

However, Idaho may be a legal battleground for more than the popularity of farming and pesticide use in that state. Soda Springs, Idaho is a major source of elemental phosphorus, which is a key Roundup ingredient, and is the only place in the western hemisphere where it is mined.

Read More

GLP, 12-02-24

https://geneticliteracyproject.org/2024/02/12/idaho-lawmakers-introduce-bill-to-curb-pesticide-lawsuits-citing-exploitation-of-the-legal-system-by-anti-chemical-activists/

California's war on plastic bag use seems to have backfired. Lawmakers are trying again

2024-02-12

It was a decade ago when California became the first state in the nation to ban single-use plastic bags, ushering in a wave of anti-plastic legislation from coast to coast.

But in the years after California seemingly kicked its plastic grocery sack habit, material recovery facilities and environmental activists noticed a peculiar trend: Plastic bag waste by weight was increasing to unprecedented levels.

According to a report by the consumer advocacy group CALPIRG, 157,385 tons of plastic bag waste was discarded in California the year the law was passed. By 2022, however, the tonnage of discarded plastic bags had skyrocketed to 231,072 — a 47% jump. Even accounting for an increase in population, the number rose from 4.08 tons per 1,000 people in 2014 to 5.89 tons per 1,000 people in 2022.

The problem, it turns out, was a section of the law that allowed grocery stores and large retailers to provide thicker, heavier-weight plastic bags to customers for the price of a dime.

"It was a conscious decision to create a pathway for a type of reusable bag that barely existed," said Mark Murray, director of Californians Against Waste, an environmental organization. "It was just emerging in

the marketplace, but it happened to be made by a couple of California companies ... which the manufacturers claimed they could certify as being reusable."

He said the bags were made of 20% recyclable material and the manufacturers said they could be recycled at the end of their "useful life. ... So we said, all right, fine. We're gonna put that specific criteria into the law."

"That experiment failed," Murray said.

"It was a gaping hole," said Mark Gold, director of Water Scarcity Solutions, Environmental Health at the Natural Resources Defense Council who worked on the original legislation — SB 270 — while he was with the organization Heal the Bay.

These "reusable" bags are made from a material known as HDPE, which is thicker and heavier than the LDPE plastic bags of yore. And although both materials can be recycled — and in commercial and agricultural settings often are recycled — they are generally not in residential and consumer settings, Murray said.

Read More

LA Times, 12-02-24

https://www.latimes.com/environment/story/2024-02-12/californias-war-on-plastic-bag-use-seems-to-have-backfired

Per- and Polyfluoroalkyl Substances (PFAS) in Pesticide and Other Packaging - EPA Actions

2024-02-15

On February 15, 2024, EPA released a new method to detect 32 PFAS directly from the walls of containers made from high-density polyethylene (HDPE). The robust and validated method allows for sensitive detection of PFAS contamination, measuring levels as low as 0.002 parts-per-billion (or 2 parts-per-trillion). This new method will allow industries that use HDPE containers and container manufacturers to test the containers before use, preventing PFAS contamination of products stored in these containers. The method also has wide applicability for other industries, as it can be modified to test for PFAS in additional solid samples such as fabric, packaging paper, and more.

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View the method for detecting PFAS in containers here: Quantitative Extraction and Analysis of PFAS from Plastic Container Walls with Cut Coupons (pdf) (417.5 KB)

In December 2023, EPA issued orders to Inhance Technologies LLC (Inhance) directing it not to produce per- and polyfluroalkyl substances (PFAS), chemicals that are created in the production of its fluorinated high-density polyethylene (HDPE) plastic containers. This action, taken under the authority of the Toxic Substances Control Act (TSCA), will help protect the public from exposure to dangerous PFAS chemicals in containers used for a variety of household consumer, pesticide, fuel, automotive and other industrial products.

Read More

US EPA, 15-02-24

https://www.epa.gov/pesticides/pfas-packaging#Actions

EUROPE

Textiles and food waste reduction: New EU rules to support circular economy

2024-02-12

The Environment Committee adopted its proposals to better prevent and reduce waste from food and textiles across the EU.

On Wednesday, MEPs in the Environment Committee adopted their position on the proposed revision of the Waste Framework Directive, by 72 votes in favour, none against and three abstentions.

More ambitious food waste reduction targets

MEPs want to increase the binding waste reduction targets proposed by the Commission to at least 20% in food processing and manufacturing (instead of 10%) and to 40% per capita in retail, restaurants, food services and households (instead of 30%), in comparison to the annual average generated between 2020 and 2022. EU countries would need to ensure that these targets are achieved at national level by 31 December 2030.

MEPs also want the Commission to evaluate the possibility and make appropriate legislative proposals to introduce higher targets for 2035 (at least 30% and 50% respectively).

Extended producer responsibility for textile products, clothing and footwear

The new rules, as adopted by MEPs, would set up extended producer responsibility (EPR) schemes, through which economic operators that make textiles available on the EU market would cover the costs for their separate collection, sorting and recycling. Member states would have to establish these schemes 18 months after the entry into force of the directive (compared to 30 months proposed by the Commission). In parallel, EU countries would need to ensure, by 1 January 2025, the separate collection of textiles for re-use, preparing for re-use and recycling.

These rules would cover textile products such as clothing and accessories, blankets, bed linen, curtains, hats, footwear, mattresses and carpets, including products that contain textile-related materials such as leather, composition leather, rubber or plastic.

Quote

Rapporteur Anna Zalewska (ECR, PL) said: "We provide focused solutions to reduce food waste, such as promoting "ugly" fruits and veggies, keeping an eye on unfair market practices, clarifying date labelling and donating unsold-but-consumable food. For textiles, we patch up loopholes by also including non-household products, carpets and mattresses, as well as sales via online platforms. We also request a textile waste reduction target, with an oversight of exported used textiles. Better infrastructure to increase separate collection should be complemented by sorting mixed municipal waste more efficiently, so that items which can be recycled are extracted before being sent to the incinerator or landfill."

Next steps

The full house is scheduled to vote on its position during the March 2024 plenary session. The file will be followed up by the new Parliament after the European elections on 6-9 June.

Read More

European Parliament, 12-02-24

https://www.europarl.europa.eu/news/en/press-room/20240212IPR17625/textiles-and-food-waste-reduction-new-eu-rules-to-support-circular-economy

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New GB active substance non-renewal decision

2024-02-24

Biocidal products must be phased off the GB market

Following the applicant's withdrawal of support under the GB BPR, a decision has been taken not to renew the following active substance approval in GB:

Acrylaldehyde (Acrolein) (CAS 107-02-8 EC 203-453-4) in product type 12

As this active substance/product type combination is no longer supported for renewal, the previously postponed expiry date to allow the renewal to be carried out is no longer relevant. Therefore, the approval expiry date has changed from 28 February 2026 to 31 January 2024.

If you hold an affected GB BPR product authorisation or Control of Pesticides Regulations (COPR) product approval, we will contact you about cancelling or revoking your authorisation or approval. You will have an opportunity to submit comments or additional information and we will take account of these when finalising our decision.

Read More

HSE, 14-02-24

https://content.govdelivery.com/accounts/UKHSE/bulletins/38a4269

Upcoming GB active substance open invitation deadlines

2024-02-14

Submit a notification by the deadline to keep active substances in the GB Review Programme

HSE has published open invitations (.pdf) to provide an opportunity for a person, company or task force/consortium to notify an intention to take up or take over the role of participant in the GB Review Programme for the following active substance/product type combinations.

Anyone wishing to support one of the active substance/product type combinations listed below in GB will need to submit a notification to HSE by the following deadlines:

- Reaction products of 5,5-dimethylhydantoin, 5-ethyl-5-methylhydantoin with chlorine (DCEMH) (CAS 89415-87-2 EC 401-570-7) in product type 11

15 February 2025

- Reaction products of 5,5-dimethylhydantoin, 5-ethyl-5-methylhydantoin with bromine and chlorine (DCDMH) (CAS n/a EC n/a) in product type 11

15 February 2025

- If a notification to take over the role of participant is not received, these active substance/product type combinations will be subject to a GB non-approval decision. This means the active substances will no longer be able to be used in biocidal products of the relevant product types in GB.

In addition articles treated with such products will no longer be able to be placed on the market in GB. HSE will provide separate updates on these where relevant.

Read More

HSE, 14-02-24

https://content.govdelivery.com/accounts/UKHSE/bulletins/38a4269

Upcoming GB active substance expiry dates

2024-02-14

Biocidal products must be phased off the GB market

The active substance/product type combinations listed below are due to expire under the GB BPR on the following dates:

- 1-[[2-(2,4-dichlorophenyl)-4-propyl-1,3-dioxolan-2-yl]methyl]-1H-1,2,4-triazole (Propiconazole) (CAS 60207-90-1 EC 262-104-4) in product type 9

31 May 2025

- Carbon dioxide (CAS 124-38-9 EC 262-104-4) in product type 15

31 May 2025

Once the approvals expire, the active substances will no longer be able to be used in biocidal products of the relevant product types in GB. In addition articles treated with such products will no longer be able to be placed on the market in GB.

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Read More

HSE, 14-02-24

https://content.govdelivery.com/accounts/UKHSE/bulletins/38a4269

REACH Update

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Guidance on the assessment of risks to bees from the use of biocides

2024-02-12

The European Commission asked ECHA to develop guidance for assessing the risks to arthropod pollinators (including bees) from the use of biocides, considering EFSA's Guidance on the risk assessment of plant protection products on bees. This Guidance Document describes how to perform a risk assessment for bees, in accordance with Article 19(1)(b)(iv) of the Biocidal Products Regulation (BPR). It proposes a tiered approach scheme for biocidal active substances for the exposure estimation in different scenarios, hazard characterisation and a risk assessment methodology covering both dietary and contact exposure. This document also provides recommendations for higher tier assessment, metabolite risk assessment and biocidal product risk assessment (mixtures). For arthropod pollinators other than bees, an overview of the literature and a database search on the ecology and sensitivity of non-bee pollinators are provided together with recommendations for further research and considerations for future development of guidance.

Read More

ECHA, 12-02-24

https://echa.europa.eu/documents/10162/2324906/guidance_on_assessment_risks_to_bees_from_biocides_en.pdf/

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Janet's Corner

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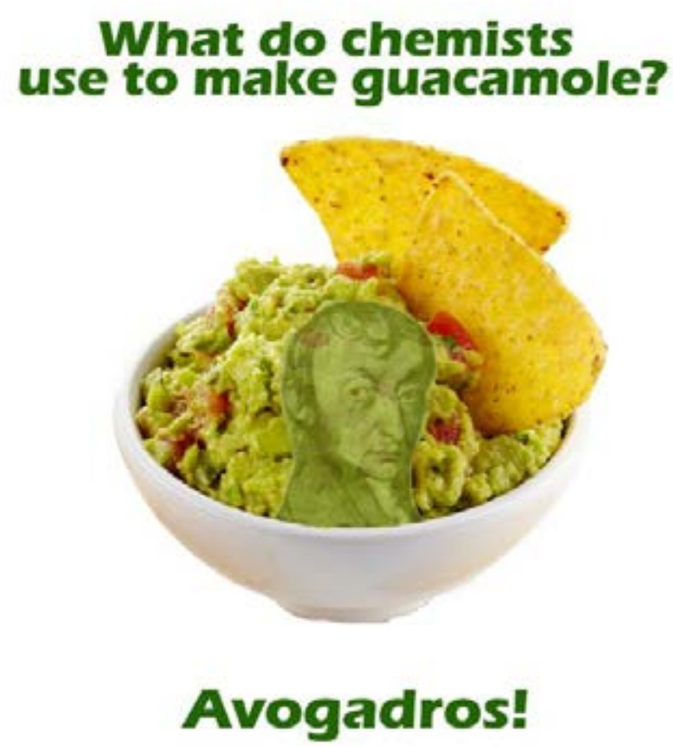
Guacamole

2024-02-23



http://www.calpaclab.com/science-jokes/

Aniline

2024-02-23

USES [2,3]

Aniline is predominantly used as a chemical intermediate. It is used in rubber accelerators and anti-oxidants, dyes and intermediates, photographic chemicals, as isocyanates for urethane foams, in pharmaceuticals, explosives, petroleum refining; and in production of diphenylamine, phenolics, herbicides and fungicides. Aniline is also used in the manufacture of polyurethanes, rubber processing chemicals, pesticides, fibres, dyes and pigments, photographic chemicals, and pharmaceuticals.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

Aniline can be formed from the breakdown of certain pollutants found in outdoor air, from the burning of plastics, or from burning tobacco. Airborne exposure to aniline may occur from breathing contaminated air, from smoking tobacco or proximity to someone who is smoking, or from being near industrial sources that use large quantities of aniline. Occupational exposure to aniline could occur in industries that use aniline to make other chemicals. In addition, small amounts of aniline may be found in some foods, such as corn, grains, rhubarb, apples, beans, and rapeseed cake (animal feed). Aniline has also been found as a volatile component of black tea. Aniline has been detected in drinking water and has also been found in surface water.

Routes of Exposure

The major routes of exposure for aniline include absorption into the body via inhalation of the vapour, through the skin and by ingestion.

HEALTH EFFECTS [4]

Acute Health Effects

Acute inhalation exposure to high levels of aniline in humans has resulted in effects on the lung, such as upper respiratory tract irritation and congestion. Aniline has been classified as very toxic in humans, with a probable oral lethal dose in humans at 50 to 500 milligrams per kilogram

Aniline, phenylamine or aminobenzene is an organic compound with the formula C6H5NH2. Consisting of a phenyl group attached to an amino group, aniline is the prototypical aromatic amine.

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body weight (mg/kg). It is considered to have high acute toxicity, based on short-term animal tests in rats.

Carcinogenicity

A study of British workers in the chemical dye industry exposed to aniline and other chemicals concluded that there was insufficient evidence to suggest that aniline itself is a cause of bladder tumours. Animal studies have demonstrated an increase in tumours of the spleen in rats exposed to aniline hydrochloride. EPA considers aniline to be a probable human carcinogen (cancer-causing agent) and has ranked it in EPA's Group B2.

Other Effects

No information is available on the reproductive or developmental effects of aniline in humans. Birth defects were observed in animals given aniline by gavage (placing the chemical experimentally in the stomachs of the animals). The total number of offspring in mice given aniline by gavage was lower than in the control group even though the average number of offspring per litter was not affected. However, some of the pregnant mice treated with aniline died during pregnancy. Survival of offspring in the aniline-treated group was decreased.

SAFETY

First Aid Measures [5]

- **Eye Contact:** Check for and remove any contact lenses. Immediately flush eyes with running water for at least 15 minutes, keeping eyelids open. Cold water may be used. Get medical attention. Finish by rinsing thoroughly with running water to avoid a possible infection.
- **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. Cold water may be used. 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.
- **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 workstation location.

The following work practices are also recommended:

- Keep locked up
- Keep away from heat.
- Keep away from sources of ignition.
- Ground all equipment containing material.
- Do not ingest.
- Do not breathe gas/fumes/ vapour/spray.
- Wear suitable protective clothing. In case of insufficient ventilation, wear suitable respiratory equipment.
- If ingested, seek medical advice immediately and show the container or the label.
- Avoid contact with skin and eyes.
- Keep away from incompatibles such as oxidising agents, metals, acids, alkalis.

Personal Protective Equipment [5]

The following personal protective equipment is recommended when handling aniline:

- Splash goggles

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- Full suit
- Vapour respirator
- Boots
- Gloves
- A self-contained breathing apparatus should be used to avoid inhalation of the product.
- NOTE: Suggested protective clothing might not be sufficient; consult a specialist BEFORE handling this product.

REGULATION

United States

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

- General Industry: 29 CFR 1910.1000 Z-1 Table -- 5 ppm, 19 mg/m3 TWA; Skin
- Construction Industry: 29 CFR 1926.55 Appendix A -- 5 ppm, 19 mg/m3 TWA; Skin
- Maritime: 29 CFR 1915.1000 Table Z-Shipyards -- 5 ppm, 19 mg/m3 TWA; Skin

ACGIH: The American Conference of Governmental Industrial Hygienists has set a Threshold Limit Value (TLV)for aniline of 2 ppm, 7.6 mg/m3 TWA; Skin; Appendix A3, Confirmed Animal Carcinogen with Unknown Relevance to Humans; BEI

NIOSH: The National Institute for Occupational Safety and Health has listed aniline as a Potential Occupational Carcinogen.

REFERENCES

1. http://en.wikipedia.org/wiki/Aniline
2. http://www.atsdr.cdc.gov/toxfaqs/tfacts171.pdf
3. http://www.epa.gov/ttn/atw/hlthef/aniline.html
4. http://www.npi.gov.au/substances/aniline/index.html
5. http://www.sciencelab.com/msds.php?msdsId=9927435
6. https://www.osha.gov/dts/chemicalsampling/data/CH_218800.html

Conversion Process Turns Greenhouse Gas Into Ethylene

2024-02-14

Engineers at the University of Cincinnati created a more efficient way of converting carbon dioxide into valuable products while simultaneously addressing climate change.

In his chemical engineering lab in UC's College of Engineering and Applied Science, Associate Professor Jingjie Wu and his team found that a modified copper catalyst improves the electrochemical conversion of carbon dioxide into ethylene, the key ingredient in plastic and a myriad of other uses.

Ethylene has been called "the world's most important chemical." It is certainly among the most commonly produced chemicals, used in everything from textiles to antifreeze to vinyl. The chemical industry generated 225 million metric tons of ethylene in 2022.

Wu said the process holds promise for one day producing ethylene through green energy instead of fossil fuels. It has the added benefit of removing carbon from the atmosphere.

"Ethylene is a pivotal platform chemical globally, but the conventional steam-cracking process for its production emits substantial carbon dioxide," Wu said. "By utilizing carbon dioxide as a feedstock rather than depending on fossil fuels, we can effectively recycle carbon dioxide."

The study was published in the journal Nature Chemical Engineering.

Wu's students, including lead author and UC graduate Zhengyuan Li, collaborated with Rice University, Oak Ridge National Laboratory, Brookhaven National Laboratory, Stony Brook University and Arizona State University. Li received a prestigious graduate student award last year from the College of Engineering and Applied Science.

The electrocatalytic conversion of carbon dioxide produces two primary carbon products, ethylene and ethanol. Researchers found that using a modified copper catalyst produced more ethylene.

"Our research offers essential insights into the divergence between ethylene and ethanol during electrochemical CO2 reduction and proposes a viable approach to directing selectivity toward ethylene," lead author Li said.

National research team led by UC professor develops more efficient system to address climate change.

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"This leads to an impressive 50% increase in ethylene selectivity," Wu said. "Ideally, the goal is to produce a single product rather than multiple ones."

Sponsored by the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy. Its Industrial Efficiency and Decarbonization Office is leading efforts to reduce fossil fuels and carbon emissions in industry wherever possible.

Li said the next step is refining the process to make it more commercially viable. The conversion system loses efficiency as byproducts of the reaction such as potassium hydroxide begin forming on the copper catalyst.

"The electrode stability must be improved for commercial deployment. Our next focus is to enhance stability and extend its operation from 1,000 to 100,000 hours," Li said.

Wu said these new technologies will help make the chemical industry greener and more energy efficient.

"The overarching objective is to decarbonize chemical production by utilizing renewable electricity and sustainable feedstock," Wu said. "Electrifying the conversion of carbon dioxide to ethylene marks a significant stride in decarbonizing the chemical sector."

Technology Networks, 14 February 2024

https://technologynetworks.com

New class of 'intramolecular bivalent glue' could transform cancer drug discovery

2024-02-21

A research team at the University's Centre for Targeted Protein Degradation (CeTPD) led by Professor Alessio Ciulli, in collaboration with the research group of Dr. Georg Winter at the Research Center for Molecular Medicine (CEMM) of the Austrian Academy of Sciences in Vienna, have defined a new class of so-called "intramolecular bivalent glue," which bind proteins—crucial to the cells that allow our bodies to function correctly—that would otherwise stay apart.

This research has been published in the journal Nature.

A breakthrough class of molecular glue identified at the University of Dundee could pave the way for a new generation of drugs to target cancers and neurodegenerative diseases.

"These findings have major implications for the entire pharmaceutical industry engaged in targeted protein degraders," said Professor Alessio Ciulli, Director of Dundee's CeTPD.

"This is particularly true for the development of drugs that target cancer, neurodegenerative diseases, and many more illnesses driven by proteins that have always been considered undruggable."

"Proteins are essential for our cells to function properly, but when these do not work correctly, the body is vulnerable to disease."

"The glue that we have been able to define is special because it first attaches itself to one protein in two places—not just one—and then recruits the second protein, effectively sandwiching the two proteins together.

"We have only been able to identify this using our Targeted Protein Degradation technology and have identified a vulnerability that can be exploited by the design of new drugs that could potentially transform treatment for cancer patients and those with other untreatable diseases."

Targeted protein degradation (TPD) is an emerging field of drug development for treating diseases that involves redirecting protein recycling systems in our cells to destroy disease-causing proteins. Most TPD strategies use small molecules—so-called degraders—to recruit these target proteins to a class of enzymes called ubiquitin E3 ligases.

The E3 tags the target protein with ubiquitin labels, which ultimately leads to the destruction of the disease-causing protein via the cellular waste bin: the proteasome.

Working with collaborators at CEMM, the Goethe University of Frankfurt, and Eisai Co. Ltd, the Japanese pharmaceutical company, the Dundee team has been able to unveil a novel mechanism of molecular gluing, different from those previously known. This new mechanism binds to two sides of the target protein instead of just one, prompting a rearrangement of the whole protein and stabilizing its previously unknown interaction with the E3 ligase.

Furthermore, the team was able to visualize, for the first time, the precise mechanism by which their compounds work and bring together the target proteins to one of these E3 ligases. Because the molecules have two heads, which latch on to two different regions within the same target protein, these have been coined "intramolecular bivalent glues."

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This world-leading work has also illuminated previously underappreciated features and properties of molecular glues, paving the way for scientists to develop a deeper understanding of glues that could allow for new classes to be discovered more rapidly.

"The impact of what we have revealed here cannot be underestimated," added Professor Ciulli. "This will cause a ripple effect throughout the pharmaceutical industry and has the potential to transform how we view drug development. I must also pay tribute to our collaborators, whose input has been crucial in achieving this seismic breakthrough."

Phys Org, 21 February 2024

https://phys.org

Revolutionary Method Uses Old Milk to Extract Gold from E-Waste

2024-02-09

Discarded electronics, known as e-waste, often contain large amounts of gold and other heavy metals. There are various methods for recovering these valuable metals. However, many methods use harmful synthetic chemicals. However, a team of researchers at ETH Zurich in Switzerland has come up with a new and innovative way to extract gold from e-waste using a surprising ingredient – old milk.

The team, led by Raffaele Mezzenga, used whey protein – a byproduct of the cheesemaking industry – to create a low-density aerogel. This spongelike material is not only cheap to make, but it also has high porosity and surface area, making it an ideal candidate for extracting gold from e-waste solutions.

The process starts by placing whey protein into an acidic solution and heating it. This causes the proteins to unravel and form strands. The solution is freeze-dried next. This process creates a lightweight puck. The puck has high porosity. You can place them on the top of a flower, explains Mohammad Peydayesh, a chemical engineer involved in the research team.

To test the gel's ability to adsorb gold from e-waste solutions containing other metals such as copper, lead, and nickel, the researchers found that it was able to remove 93% of the gold while only removing less than 10% of any other metal. In comparison, activated carbon – another commonly

Old Milk Miracle – You Won't Believe How This Ordinary Kitchen Ingredient Can Extract Gold from Your Old Electronics!

used adsorption method for recovering gold – only adsorbed about 60 mg per gram from an e-waste mixture.

What happens when this protein sponge is tested on actual e-waste? The team dissolved computer motherboards in aqua regia (a mix of nitric acid and hydrochloric acid) and found that each gram of aerogel was able to snatch 190 mg of gold. When the aerogel is burned, it releases the gold. This gold appears as a small piece of metal. It is about 91% pure. This purity level is equivalent to 21 to 22 carats.

It was really exciting to find this nugget in the ashes, recalls Peydayesh. Not only does this method present an improvement over traditional methods, but it also has a lower environmental impact. Activated carbon requires a lot of energy to create, making it less sustainable than using old milk.

The team is exploring other proteins from food waste. These could help recycle rare earth metals. We can simultaneously address the global waste of food and e-waste to produce something really precious, says Peydayesh.

So next time you pour out that old milk, think twice before throwing it away – it could hold more value than you think!

ENTECH, 9 February 2024

https://entechonline.com

New Analysis Method Can Detect Forever Chemicals in Under Three Minutes

2024-02-09

Per- and polyfluoroalkyl substances (PFAS) used to be household staples, being used in a wide range of grease-proof, water-proof and stain-resistant products. Now, these compounds are more commonly known as "forever chemicals" for their extreme persistence in the environment. Unable to breakdown naturally, these chemicals accumulate and spread over time.

Detecting the presence of PFAS in a given sample is typically a very time-consuming process, requiring lengthy sample preparation. But a new laboratory method developed by chemists at the New Jersey Institute of Technology (NJIT) promises to detect traces of PFAS in just three minutes or less.

The new lab method can detect traces of PFAS from food packaging, water and soil samples in three minutes or less.

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The technique has been demonstrated on samples of drinking water, tap water, wastewater, paper food packaging and soil samples in a new paper, published in the Journal of Hazardous Materials.

A rapid lab test for PFAS

PFAS testing is a tricky business. Due to their extreme persistence, PFAS tests need to be carried out on a wide variety of different sample types. Complex samples, such as soil, will present extra challenges as they are likely to contain other minerals and microorganisms that will complicate analysis.

To cope with this complexity, traditional PFAS analysis normally involves some kind of solid phase extraction (SPE) or liquid-liquid extraction (LLE) step to preconcentrate samples prior to analysis. Analysis is most commonly done with liquid chromatography with tandem mass spectrometry (LC-MS/MS) or a similar technique.

Practically, this analysis works very well. But the intricate sample preparation and liquid chromatography steps required are very time consuming.

The new method proposed by the NJIT researchers is based on an ionization technique called paper spray mass spectrometry (PS-MS), a variant on electrospray ionization. In PS-MS, a few microliters of the sample and solvent are applied to a piece of filter paper. With the sample mounted on the wetted paper, a high voltage is applied. This creates an electrospray-like event, sending ions of the analyte towards the mass spectrometer for analysis.

"PFAS can be ionized and rapidly detected by a high-resolution mass spectrometer, which gives a clear view of each PFAS species present and the degree of contamination down to a parts-per-trillion (ppt) level," said corresponding author Hao Chen, a professor of chemistry and environmental science at NTIJ. "For more complex matrices like soil, we've applied a related method called desalting paper spray mass spectrometry (DPS-MS) that washes away salts which normally suppress the ion signal of PFAS. Together, they greatly improve our ability to detect these compounds."

"Our limit of detection for PFAS is roughly 1ppt [parts per trillion]. For context, this amount has been likened to a drop of water in 20 Olympic-sized swimming pools," added first author Md Tanim-Al Hassan, a PhD student in chemistry at NJIT.

Rapid testing of water, soil and food packaging

In tests on soil samples, the team were able to identify two species of PFAS from as little as 40 milligrams of soil in under three minutes.

To demonstrate the technique's use in water analysis, the researchers tested samples of local tap water alongside the filtered fountain water available at the university. The PS-MS technique detected traces of perfluorooctanoic acid (PFOA) – one of the most widely studied PFAS chemicals – in the tap water in just under two minutes. No PFAS compounds were detected in the filtered water.

Technology Networks, 9 February 2024

https://technologynetworks.com

Run out of butter or eggs? Here's the science behind substitute ingredients

2024-02-19

Unless you can immediately run to the shops, this can leave you scrambling for a substitute that can perform a similar function. Thankfully, such substitutes can be more successful than you'd expect.

There are a few reasons why certain ingredient substitutions work so well. This is usually to do with the chemistry and the physical features having enough similarity to the original ingredient to still do the job appropriately.

Let's delve into some common ingredient substitutions and why they work—or need to be tweaked.

Oils versus butter

Both butter and oils belong to a chemical class called lipids. It encompasses solid, semi-solid and liquid fats.

In a baked product the "job" of these ingredients is to provide flavor and influence the structure and texture of the finished item. In cake batters, lipids contribute to creating an emulsion structure—this means combining two liquids that wouldn't usually mix. In the baking process, this helps to create a light, fluffy crumb.

One of the primary differences between butter and oil is that butter is only about 80% lipid (the rest being water), while oil is almost 100% lipid. Oil creates a softer crumb but is still a great fat to bake with.

It's an all too common situation—you're busy cooking or baking to a recipe when you open the cupboard and sud-denly realize you are missing an ingredient.

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You can use a wide range of oils from different sources, such as olive oil, rice bran, avocado, peanut, coconut, macadamia and many more. Each of these may impart different flavors.

Other "butters", such as peanut and cashew butter, aren't strictly butters but pastes. They impart different characteristics and can't easily replace dairy butter, unless you also add extra oil.

Aquafaba or flaxseed versus eggs

Aquafaba is the liquid you drain from a can of legumes—such as chickpeas or lentils. It contains proteins, kind of how egg white also contains proteins.

The proteins in egg white include albumins, and aquafaba also contains albumins. This is why it is possible to make meringue from egg whites, or from aquafaba if you're after a vegan version.

The proteins act as a foam stabilizer—they hold the light, airy texture in the product. The concentration of protein in egg white is a bit higher, so it doesn't take long to create a stable foam. Aquafaba requires more whipping to create a meringue-like foam, but it will bake in a similar way.

Another albumin-containing alternative for eggs is flaxseed. These seeds form a thick gel texture when mixed with a little water. The texture is similar to raw egg and can provide structure and emulsification in baked recipes that call for a small amount of egg white.

Lemon plus dairy versus buttermilk

Buttermilk is the liquid left over after churning butter—it can be made from sweet cream, cultured/sour cream or whey-based cream. Buttermilk mostly contains proteins and fats.

Cultured buttermilk has a somewhat tangy flavor. Slightly soured milk can be a good substitute as it contains similar components and isn't too different from "real" buttermilk, chemically speaking.

One way to achieve slightly soured milk is by adding some lemon juice or cream of tartar to milk. Buttermilk is used in pancakes and baked goods to give extra height or volume. This is because the acidic (sour) components of buttermilk interact with baking soda, producing a light and airy texture.

Buttermilk can also influence flavor, imparting a slightly tangy taste to pancakes and baked goods. It can also be used in sauces and dressings if you're looking for a lightly acidic touch.

Honey versus sugar

Honey is a complex sugar-based syrup that includes floral or botanical flavors and aromas. Honey can be used in cooking and baking, adding both flavor and texture (viscosity, softness) to a wide range of products.

If you add honey instead of regular sugar in baked goods, keep in mind that honey imparts a softer, moister texture. This is because it contains more moisture and is a humectant (that is, it likes to hold on to water). It is also less crystalline than sugar, unless you leave it to crystallize.

The intensity of sweetness can also be different—some people find honey is sweeter than its granular counterpart, so you will want to adjust your recipes accordingly.

Gluten-free versus regular flour

Sometimes you need to make substitutions to avoid allergens, such as gluten—the protein found in cereal grains such as wheat, rye, barley and others.

Unfortunately, gluten is also the component that gives a nice, stretchy, squishy quality to bread.

To build this characteristic in a gluten-free product, it's necessary to have a mixture of ingredients that work together to mimic this texture. Common ingredients used are corn or rice flour, xanthan gum, which acts as a binder and moisture holder, and tapioca starch, which is a good water absorbent and can aid with binding the dough.

Phys Org, 19 February 2024

https://phys.org

Pre-organising antibiotic structure could aid fight against resistance

2024-02-22

Lincosamide antibiotics, such as clindamycin, work by binding to the bacterial ribosome, arresting protein synthesis. However, bacterial evolution has produced many ribosome modifications that confer resistance by reducing the binding affinity of these antibiotics, rendering them ineffective.

To find a way to overcome this challenge, the researchers, who were from Andrew Myers' research group in the department of chemistry and

A novel synthetic antibiotic with a structure preorganised for optimal ribosomal binding has been shown to be effective against several multi-drug resistant strains of bacteria.

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chemical biology at Harvard University in the US, took a newly developed lincosamide that they had previously reported – iboxamycin – and examined its conformation while bound to the bacterial ribosome.

'We observed atoms that were quite close to each other and decided that it might be feasible to link those together, resulting in a pre-organised or pre-rigidified conformation that most closely resembles how it will look when bound to the bacterial ribosome,' explains Kelvin Wu, a chemistry graduate student in Myers' group and first author on the study.

'If a molecule is very flexible with many rotatable bonds, it incurs a significant entropy cost to freeze those bonds when the molecule binds to the bacterial ribosome,' Wu says. 'By pre-organising a molecule into its preferred binding conformation, you can reduce the entropy cost of binding to its target which then translates to an increase in free energy and a stronger binding interaction.'

Conformational restriction of the aminooctose residue of iboxamycin through transannular macrocyclisation led to the formation of cresomycin, a new antibiotic pre-organised for binding to the bacterial ribosome. Results from in vitro studies suggested that cresomycin had efficacy against both Gram-positive and Gram-negative bacteria, including those on the World Health Organization's priority pathogen list, such as carbapenem-resistant Escherichia coli and Pseudomonas aeruginosa. This efficacy was also demonstrated in in vivo studies using mouse models.

Stephen Cochrane, reader in organic chemistry and chemical biology at Queen's University Belfast, describes cresomycin as a 'very promising lead'. 'It's a nice use of rational design coupled with computational aids to create a new analog of lincomycin,' he adds. 'It's not a new class of antibiotic because it is still based on something that's operating by the same mechanism but it's a nice use of that approach to give us something new.'

'The positive with any new antimicrobial compound that's active against current resistant strains is that we have a new weapon in the arsenal. It's also overcoming known resistance mechanisms for macrolides and lincosamide antibiotics – such as lincomycin or erythromycin – which kill bacteria by binding to the ribosome.'

Cochrane highlights several limitations which, he says, would need to be addressed before the compound could make its way to the clinic. 'The big glaring one is the effort required to access it through total synthesis – the whole process, at least by my calculations, is approximately 0.8% yield for approximately 25 steps. And some of these steps use toxic reagents,

extremely cold temperatures, chiral auxiliaries etc – so as it stands, it would need a lot of modifications and optimisations to be something that could be scaled.'

Study author Ben Tresco acknowledge that the current synthesis route for cresomycin is difficult to scale up. 'Once we know that these compounds work, we spend a lot of time developing what we'd consider a scalable synthesis,' he explains. 'I'm happy to say that we've been successful in this effort – we now have an entirely different route that allows us to access these really complex molecules on multi-gram scale.'

Cochrane also says that to 'future proof' the compound it would be important to investigate the likelihood of resistance mechanisms developing over a longer time frame than was tested in the study.

On 13 February, the Combating Antibiotic-Resistant Bacteria Biopharmaceutical Accelerator announced that Myers' group will receive $1.2 million (£950,000) in funding to develop a series of enhanced oral antibiotics that directly target a range of antibiotic-resistant bacteria which cause serious lower respiratory tract and skin and soft tissue infections.

Chemistry World, 22 February 2024

https://chemisrtyworld.com

A test battery for assessing the ecotoxic effects of textile dyes

2018-08-01

The textile dyeing industry is one of the main sectors contributing to environmental pollution, due to the generation of large amounts of wastewater loaded with dyes (ca. 2–50% of the initial amount of dyes used in the dye baths is lost), causing severe impacts on human health and the environment. In this context, an ecotoxicity testing battery was used to assess the acute toxicity and genotoxicity of the textile dyes Direct Black 38 (DB38; azo dye) and Reactive Blue 15 (RB15; copper phthalocyanine dye) on different trophic levels. Thus these dyes were tested using the following assays: Filter paper contact test with earthworms (Eisenia foetida); seed germination and root elongation toxicity test (Cucumis sativus, Lactuca sativa and Lycopersicon esculentum); acute immobilization test (Daphnia magna and Artemia salina); and the Comet assay with the rainbow trout gonad-2 cell fish line (RTG-2) and D. magna. Neither phytotoxicity nor significant effects on the survival of E. foetida

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were observed after exposure to DB38 and RB15. Both dyes were classified as relatively non-toxic to D. magna (LC50 > 100 mg/L), but DB38 was moderately toxic to A. salina with a LC50 of 20.7 mg/L. DB38 and RB15 induced significant effects on the DNA of D. magna but only DB38 caused direct (alkaline comet assay) and oxidative (hOGG1-modified alkaline comet assay) damage to RTG-2 cells in hormetic responses. Therefore, the present results emphasize that a test battery approach of bioassays representing multiple trophic levels is fundamental in predicting the toxicity of textile dyes, aside from providing the information required to define their safe levels for living organisms in the environment.

Introduction

The textile industry plays an important role in the economy of many countries, providing a vast range of colored fabrics for marketing, but its manufacturing activities pose challenges for environmental management, since large amounts of synthetic dyes, resistant to conventional wastewater treatments, are daily released into the environment [[1], [2], [3], [4], [5], [6], [7]]. The amount of dye that is released into the textile effluents may vary from 2% to 50% of the initial dye concentration [3,8].

Thus dye-based toxicity has been investigated over the years in order to identify hazardous dyes and, consequently, to protect human health and the environment [[3], [4], [5],[9], [10], [11], [12], [13], [14], [15]]. However, most of the studies on dye toxicity have focused on humans, and safe thresholds to protect environmental organisms are not available for most of the dyes commonly used in textile dyeing [6,14]. For example, Direct Black 38 (DB38) is an azo dye classified as carcinogenic to humans due to its biotransformation to benzidine [[16], [17], [18]], but there is a lack of data on its impact to terrestrial and aquatic organisms. Recently, Oliveira and co-authors [5] pointed out that care should be taken in discharging DB38-containing wastewater, since this dye has been shown to be embryotoxic for the zebrafish model. Reactive Blue 15 (RB15), a copper-phthalocyanine dye, is toxic for the bacteria, tadpoles and embryo fish models [5,19,20]. The identification of its toxicity for species covering other trophic levels is relevant to gather additional ecotoxicological knowledge, and hence determine its safe level to protect the environment. Species-specific toxicity has already been demonstrated for Reactive Red 120, which reinforces the use of a multiple trophic levels eco-tests approach to accurately predict the ecotoxic effects of textile dyes [4].

One of the core missions of ecotoxicology is to understand the underlying mechanisms behind pollutants that can disturb the normal

physiological condition of biological systems, in order to prevent adverse outcomes resulting from them [21]. Thus short-term assays are useful ecotoxicological tools for estimating the acute toxicity caused by environmental chemicals.

Plants are the foundation of terrestrial and aquatic ecosystems, acting as primary producers in the food chain [22]. Thus, phytotoxicity tests are a vital part of ecotoxicological assessment, the seed germination and root elongation test being the simplest one, and representative of the action of the toxicant at the first interface of the developing plant (seed) and its environment [23]. Earthworms (terrestrial invertebrate) are considered to be suitable indicator species for ecotoxicological assessment, since they may represent 60–80% of the total soil biomass and play crucial roles in soil functioning (e.g. aeration, moisture content, nutrient cycling), apart from being sensitive to low toxicant concentrations [24,25]. Thus the acute earthworm toxicity test using Eisenia foetida or Eisenia andrei has been recommended for detecting potential soil toxicants by both regulatory agencies and environmental monitoring programs [26].

Daphnia, also called "water flea", is a planktonic invertebrate organism inhabiting freshwater ecosystems. Since Daphnia are sensitive to several chemicals and easily cultured under laboratory conditions, they are considered to be very useful bioindicators in ecotoxicology [27]. The acute immobilization test [28] with daphnids is used to detect water toxicants [29,30]. Artemia spp. (brine shrimp) is a major taxon in many hypersaline biotypes throughout the world, feeding primarily on phytoplankton and being an important primary consumer [31]. They present several advantages, such as a short life cycle and adaptability to wide ranges of salinity, which have contributed to increasing the use of brine shrimps in ecotoxicological studies [31,32].

Fish are also currently used in the assessment of chemical toxicity in aquatic environments, since they are the most diverse group of vertebrates found in this ecosystem [33]. Toxicological research on fish is largely based on in vivo studies. However, today there are a number of economic, scientific and ethical reasons for supporting efforts to develop and apply in vitro assays in aquatic ecotoxicology as alternative tools to animal testing [34,35]. Fish cell lines are of particular interest since they represent standardized systems that can be carried out in a controlled environment, giving fast, affordable and ethically eligible results [[34], [35], [36], [37]]. Among the fish cell lines available so far, the RTG-2 cell line derived from rainbow trout (Oncorhynchus mykiss) gonadal tissue has

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been successfully used in assessing aquatic genotoxicants [[38], [39], [40], [41], [42], [43]].

Considering that textile dyes are often discarded into aquatic environments and that their ecotoxicological effects are not completely known, the aim of this work was to assess the acute toxicity and genotoxicity of the textile dyes Direct Black 38 (DB38; azo dye) and Reactive Blue 15 (RB15; copper phthalocyanine dye). For this purpose, an ecotoxicity testing battery approach composed of multiple trophic levels test systems was used, since dyes, like other chemicals, can display species-specific toxicity.

Section snippets

Tested compounds

The dyes Direct Black 38 (DB38; Chlorazol Black E; purity ≥ 45%; CAS No. 1937-37-7) and Reactive Blue 15 (RB15; Turquoise Blue; purity 35%; CAS No.: 12225-39-7) were purchased from Sigma-Aldrich (St Louis, MO, USA). The chemical structure of each dye is presented in Fig. 1. For all ecotoxicity assays, the dye solutions were prepared in distilled water or test medium (i.e., culture medium) used for culturing each test organism, and without addition of solvents.

Seed germination and root elongation toxicity test

Lettuce (Lactuca sativa), cucumber (…

Phytotoxicity

During textile processing, inefficiencies in dyeing result in large amounts of the dyestuffs being directly lost to the wastewater [[3], [4], [5]]. These compounds can be released into surface waters or enter terrestrial systems when sewage effluent is employed for irrigation or where sewage sludge is applied as a fertilizer to agricultural lands [26]. Thus, considering this fact, the present study investigated the ecotoxicity of two textile dyes, DB38 and RB15, on non-target organisms…

Conclusions

Taken together, the present findings showed that the DB38 and RB15 dyes caused acute toxicity and genotoxicity for aquatic organisms, but caused no concerns with respect to terrestrial ecosystems, since phytotoxicity and earthworm toxicity were not observed. DB38 was the most toxic dye, due to its lethal toxicity on A. salina and capacity to induce DNA damage in D.

magna and RTG-2 cells. In addition, the authors attempted to carry out ecotoxicity testing within the concentration ranges of the

Conflicts of interest

The authors declare there are no conflicting interests.

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https://sciencedirect.com

AI-assisted robot lab develops new catalysts to synthesize methanol from CO_2

2024-02-20

Catalysts are chemistry's hard-working little helpers. They accelerate reactions and reduce the energy required for a reaction to take place. The more specific and effective a catalyst is, the more effectively any undesirable side reactions are suppressed.

In nature, enzymes have the job of specifically boosting the required metabolic processes from among the almost infinite reaction possibilities of the chemical soup within cells. In chemical plants, metal catalysts are usually employed to increase product yield.

The researchers working on the Swiss Cat+ technology platform at ETH Zurich, led by Paco Laveille, have now developed a fully digitalized and automated method that enables them to find new and better metal catalysts much faster than before. Their process consists of a combination of artificial intelligence (AI) for calculating promising catalyst compositions and an automated synthesis and test laboratory.

With this infrastructure, it took the team less than six weeks to successfully develop about 150 catalysts compositions for producing methanol from CO2. The best catalysts are cost-effective and exhibit high conversion

Artificial intelligence and automated laboratory infrastructure are massively accelerating the development of new chemical catalysts. With these tools, researchers at ETH Zurich are developing catalysts for efficiently and cost-effectively synthesizing the energy source methanol from CO2.

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rates with a low proportion of byproducts. "This new method saves a huge amount of time," Laveille says. "With a conventional approach, our experiments would have taken years."

The researchers have published two papers on their method. The first was published last year in CHIMIA and the second this week in Chem Catalysis.

Methanol is regarded as one of the key elements for a sustainable hydrocarbon economy. A close chemical relative of ethanol (i.e., drinking alcohol), the substance can be used both as a fuel and as a raw material for the production of organic compounds such as medicines, plastics or paints.

Because it is a liquid, methanol is much easier to transport and store than gaseous hydrogen and methane, two other sources of energy. What's more, using methanol in the existing supply infrastructure and engines of today's petrol technology requires only minor modifications.

Narrowing down the possibilities through clever preselection

In the search for optimum catalysts for methanol production, there's one big problem: Theoretically, atoms can be combined in an almost infinite number of ways to form a catalyst. "The chemical space in which we're searching for catalysts comprises around 1020 possibilities—that's one hundred billion billion. So we're literally looking for a needle in the chemical haystack," explains Christophe Copéret, a professor at the Laboratory of Inorganic Chemistry at ETH Zurich and co-initiator of the Swiss Cat+ project.

To narrow down the huge range of possibilities, the researchers made a preselection based on experience and economic requirements. A catalyst that can be used on a large scale needs to be not only effective but also inexpensive. For that reason, the main active ingredients for the catalyst were limited to three comparatively cheap metals: iron, copper and cobalt.

In addition to these main metals, the researchers considered three elements that are traditionally added to catalysts in small quantities for the purposes of doping, as well as potassium, which is also contained in many catalysts. As to carrier materials, the researchers limited themselves to four typical metal oxides. Multiplied by the different mixing ratios, this still resulted in 20 million possible combinations.

Taking iterative steps with AI-supported statistics

At this point, the researchers brought an AI algorithm into play that uses what is known as Bayesian optimization to find the best possible solutions. This special form of statistics is particularly suitable when only a small amount of data is available. Unlike in classical statistics, the probability doesn't derive from the relative frequency as calculated from numerous experiments. Instead, the calculation takes into account the probability that can be expected based on the current state of knowledge.

In the initial round, the algorithm randomly selected 24 catalyst compositions that met the specifications drawn up for the purposes of limiting the complexity. These catalysts were produced directly using the Swiss Cat+ automated laboratory infrastructure and then tested.

Delivering lots of highly reliable results quickly

The results of this initial selection served the researchers as the starting point for an AI prediction; the catalyst compositions thus predicted were in turn automatically synthesized and tested. For this first demonstration test, the scientists had their integrated system complete a total of six such rounds.

The fact that the results improved between rounds not in a linear fashion, but rather by leaps and bounds, was entirely intentional: Not only does the algorithm optimize the results of earlier rounds, it also includes an exploratory component that feeds completely new compositions into each round and learns about the chemical space. This is how the researchers prevented the calculations from getting stuck in an optimization dead end among all the possibilities.

Generating data beyond petrochemicals

In this first project, though, the researchers' primary concern wasn't to come up with the best possible catalyst for methanol synthesis. "At present, knowledge about catalysts for fuel production is based predominantly on expertise from the oil industry," Copéret says. "When it comes to reactions for use in the sustainable energy industry, reliable data is still largely lacking."

However, AI algorithms and human research intelligence need that data before they can search in a more targeted way in the vast space of chemical possibilities. "And that's precisely the kind of high-quality,

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reproducible data our AI-assisted robot laboratory now delivers. It's certain to take catalyst research a long way forward," Laveille adds.

Phys Org, 20 February 2024

https://phys.org

Cocaine Addiction Drug Could Pave Way for Colon Cancer Treatment

2024-02-14

A new, cutting-edge study from the University of Ottawa (uOttawa) has found vanoxerine, a drug initially developed for the treatment of cocaine addiction, could impede advanced colorectal cancer stem cells by essentially re-wiring critical gene networks.

This new research published in Nature Cancer led by Dr. Yannick Benoit, Principal Investigator and Associate Professor in the Department of Cellular and Molecular Medicine (Faculty of Medicine) at uOttawa, has revealed that vanoxerine plays an entirely unexpected mechanism in cancer.

Vanoxerine, a drug initially developed to treat cocaine addiction, has also shown promise for advanced colon cancer.

The investigators observed that vanoxerine packs a powerful punch when suppressing cancer stem cell activity in colon cancer patients' tissues and in tumours implanted in laboratory animals. It interferes with a protein that transports dopamine, the brain chemical involved in sensations of pleasure and reward, and represses an enzyme dubbed G9a in colorectal tumours.

"Notably, the tumours treated with vanoxerine become more susceptible to attack by the immune system due to the reactivation of ancient viral DNA fragments accumulated in our genome throughout evolution. This finding is quite significant, considering that colorectal tumours tend to show poor response to standard immunotherapy," says Dr. Benoit, who was one of six national winners of the Gairdner Foundation's 2022 Early Career Investigator competition.

A silent killer

Colorectal cancer - when cells grow and divide uncontrollably in the colon or rectum - is the world's second leading cause of cancer-related deaths and is considered a "silent cancer" since it typically doesn't cause symptoms during early stages. While the risks increase with age, new statistics show an alarming increase among younger adults.

Because it's frequently diagnosed at advanced stages when treatment options are few, it is imperative to discover new methods of beating back colorectal cancer cells and tumours. When seeking a drug safely tested in patients, the most promising option turned out to be vanoxerine, a dopamine reuptake inhibitor.

The research team observed such minimal toxicity from vanoxerine treatments when testing in healthy human and mouse tissues that Dr. Benoit says their work potentially floats "a safe way to eliminate cancer stem cells in colorectal tumours without harming the 'good stem cells' in the body's organs."

New and promising treatment

While prevention and early detection remain the best weapons against colorectal cancer, these highly compelling findings may pave the way for a new and promising treatment option for patients struggling with advanced disease.

"For those unfortunate people diagnosed with advanced and aggressive forms of colorectal cancer, we profoundly hope our work can lead to the development of powerful options for treatment in the future and substantially increase their survival chances," says Dr. Benoit.

Roots of collaboration

The study was strongly collaborative, benefitting from expertise across the uOttawa Faculty of Medicine's broad research ecosystem.

The first author is Christopher Bergin, a recent PhD graduate from Dr. Benoit's lab who methodically tested vanoxerine for its anti-cancer stem cell properties in patient-derived organoids. Dr. Rebecca Auer, scientific director of The Ottawa Hospital's Cancer Therapeutics Program, provided access to colorectal cancer patients' tissues. Dr. Mario Tiberi and Dr. Michele Ardolino provided critical insights and expertise.

While working on this study, Dr. Benoit's lab hosted Dr. Tanguy Fenouil, a gastrointestinal pathologist from France whose collaborative work was key.

Technology networks, 14 February 2024

https://technologynetworks.com

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You may be inhaling dangerous levels of chemicals thanks to your shampoo

2023-12-07

The new research, published in the journal Environmental Science & Technology, found that several chemicals commonly emitted by hair care products linger in the air much longer after use.

Researchers, including those from Purdue University in the US, say a person can inhale up to 17 mg of potentially harmful chemicals in a single hair care session in their home.

"We found the results to be extremely alarming. We did not expect to see such significant emissions of volatile chemical mixtures from off-the-shelf hair care products during typical hair care routines," study co-author Nusrat Jung said.

One of the chemicals decamethylcyclopentasiloxane, or D5 siloxane – commonly found in many personal care products – "has been found to lead to adverse effects on the respiratory tract, liver and nervous system of laboratory animals," scientists warn.

"The use of the chemical in wash-off cosmetic products has already been restricted in the European Union because of this," Dr Jung said

"Many of these products are scented, too, and some of the chemicals used to make these fragrances are potentially dangerous to inhale as well," she added.

While previous research on animals has shown that the D5 siloxane chemical is "very persistent" in the environment and can accumulate in the body, "there is little information on its human impact," scientists say.

"So we really have no idea to what extent the threat these chemicals pose when inhaled over a long period of time," Dr Jung said.

While there have been tests into chemicals present in some types of "wash-off" products like shampoos, researchers say almost no studies exist for "leave-on" products like hair gels, oils, creams, waxes, and sprays.

Applying high heat to these chemicals such as from curling irons and hair straighteners can further release chemicals into the air, scientists say.

"In urban environments, this is especially significant as you will have hundreds – even thousands – of homes ventilating out potentially harmful

People routinely using hair care products may be inhaling dangerous levels of chemicals potentially harmful to their health, an alarming new study warns.

chemicals into the urban atmosphere all in a short span of time as people get ready for work and school in the morning," Dr Jung said.

Scientists say the "best solution" is to "simply not use these products".

The next best thing, according to Dr Jung, is to have an exhaust fan running when using the products to minimise the amount of chemicals inhaled.

"Our model shows that turning on the bathroom exhaust fan can reduce D5 inhalation exposures by over 90 per cent," she said.

"The effects on people and the planet need to be studied further and regulatory action needs to be taken," Dr Jung added.

The Independent, 7 December 2023

https://independent.co.uk

European Commission to consult on bisphenol A ban in food packaging

2024-02-15

The public consultation began on 9 February and is open until 8 March. The commission will then seek approval for the proposal by member states.

'The prohibition of BPA will consequently result in business operators needing to identify substances, in particular other bisphenols and their derivatives, to replace BPA in the food contact materials and articles where it is currently used,' the commission's draft proposal reads.

BPA is used in everything from plastic and metal food containers to reusable water bottles and drinking water pipes.

The commission is proposing that BPA be barred from food contact materials with a three-year transition period for varnishes, coatings and professional food production equipment. The phase in for all other uses would be 18 months, with exemptions for the disodium salt of BPA to manufacture polysulfone resins for plastic food contact membranes, as well as for continued synthesis of bisphenol A diglycidyl ether – a compound that can be used to manufacture epoxy-based varnishes and coatings that are already restricted under a separate regulation.

A few months after Efsa's finding last year, the European Environment Agency warned that up to 100% of people taking part in EU human biomonitoring study from 11 European countries were likely exposed to BPA above safe health levels, describing public exposure to the chemical as 'well above' acceptable safety levels.

Chemistry World, 15 February 2024

https://chemistryworld.com

Ultra-high density hydrogen storage holds twice as much as liquid H2

2024-02-24

Hydrogen is finding plenty of applications as a clean fuel – in trucking and commercial vehicles, short range aviation and shipping, for example, where it carries considerably more energy per weight and volume than lithium batteries and can deliver superior range figures and quick

The European Commission is proposing a ban on the use of the endocrine disruptor bisphenol A (BPA) in food contact materials, including plastic and coated packaging.

refueling. You can burn it more or less like gasoline, or run it through a fuel cell to generate electric power.

It has the highest energy per mass of any fuel, but it's a pain to store. Keep it in gas tanks and you'll need some 700 atmospheres' worth of compression. Keep it as a liquid, and you'll need to maintain cryogenic temperatures just 20 degrees above absolute zero. And even when squashed into a supercooled liquid, it might be lightweight, but it takes up a surprising and inconvenient amount of volume, making it both energy-hungry and tough to package where space is an issue.

Now, Korean researchers say they've created a material that stores hydrogen at double the density of its cryogenic liquid form. "Our innovative material represents a paradigm shift in the realm of hydrogen storage, offering a compelling alternative to traditional approaches," said Hyunchul Oh, from the Ulsan National Institute of Science and Technology (UNIST), lead author on this new research.

As a molecule, hydrogen can physically adsorb into a porous material in a process called physisorption. Highly porous materials have previously demonstrated the ability to store a large amount of hydrogen per unit mass, but they've struggled to store a lot of energy within a small volume.

Until now. The team synthesized nanoporous magnesium borohydride ($Mg(BH_4)_2$), a framework with partially negatively-charged hydrogen atoms forming the nanopore's inner surface, enabling the uptake of hydrogen and nitrogen. Although both nitrogen and hydrogen can enter the pores, the researchers found that the gas uptake for hydrogen was larger by a factor of three as both occupy different adsorption sites in the pores.

The high hydrogen density in the small pores, the researchers observed, was due to the anisotropic (direction-dependent) shape of the hydrogen molecules normally seen as close-packed spheroids at near-ambient pressures. The material stored a cluster of five hydrogen molecules in a 3D arrangement, improving volumetric capacity.

They found that $Mg(BH_4)_2$ could store an unprecedented 144 g of hydrogen per liter of pore volume, as compared to the 70.8 g/L achieved by cryogenic liquid H_2 – or even the 86 g/l you get from solid hydrogen.

The researchers say their findings address critical challenges in large-scale hydrogen storage and enhance the efficiency and economic viability of hydrogen.

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Will this be the solution for hydrogen-powered aircraft? Possibly not. As ZeroAvia's Val Miftakhov explained to us several years ago, liquid H_2 systems in an aviation setting can achieve a hydrogen mass fraction around 30%, with the other 70% of the weight added by the tanks and cryo-cooling gear. This nanopore storage material, according to the study, delivers a mass fraction of 21.7% – so it carries twice the energy per weight that gaseous H_2 in tanks does, but a cryogenic liquid system will be lighter.

On the other hand, it could definitely play a part in long-haul shipping or trucking, where weight is less of an issue and volume is at more of a premium. And certainly, it seems like the best method yet for static energy storage situations, in which hydrogen could be used more or less like a battery.

We'd like to know more about how it's released, what kinds of temperatures and pressures it works under, and what the round-trip energy loss might be of storing hydrogen this way, but it certainly seems like a groundbreaking development in the field.

New Atlas, 24 February 2024

https://newatlas.com

Dopamine's Role in Movement Is More Important Than We Thought

2024-02-20

Imagine the act of walking. It's something most able-bodied people do without a second thought. Yet it is actually a complex process involving various neurological and physiological systems. PD is a condition where the brain slowly loses specific cells, called dopamine neurons, resulting in reduced strength and speed of movements. However, there's another important aspect that gets affected: the length of actions. Someone with PD might not only move more slowly but also take fewer steps in a walking sequence or bout before stopping. This study shows that dopamine signals directly affect the length of movement sequences, taking us a step closer to unlocking new therapeutic targets for enhancing motor function in PD.

"Dopamine is most closely associated with reward and pleasure, and is often referred to as the 'feel-good' neurotransmitter", points out Marcelo Mendonça, the study's first author. "But, for dopamine-deficient individuals with PD, it's typically the movement impairments that most impact their quality of life. One aspect that has always interested us is the concept of

Dopamine, a chemical messenger in the brain, is mostly known for its role in how we experience pleasure and reward.

lateralisation. In PD, symptoms manifest asymmetrically, often beginning on one side of the body before the other. With this study, we wanted to explore the theory that dopamine cells do more than just motivate us to move, they specifically enhance movements on the opposite side of our body".

Shedding Light on the Brain

To this end, the researchers developed a novel behavioural task, which required freely-moving mice to use one paw at a time to press a lever in order to obtain a reward (a drop of sugar water). To understand what was happening in the brain during this task, the researchers used one-photon imaging, similar to giving the mice a tiny, wearable microscope. This microscope was aimed at the Substantia nigra pars compacta (SNc), a dopamine-rich region deep within the brain that is significantly impacted in PD, allowing the scientists to see the activity of brain cells in real-time.

They genetically engineered these mice so that their dopamine neurons would light up when active, using a special protein that glows under the microscope. This meant that every time a mouse was about to move its paw or succeeded in getting a reward, the scientists could see which neurons were lighting up and getting excited about the action or the reward.

Observing these glowing neurons, the discoveries were, quite literally, illuminating. "There were two types of dopamine neurons mixed together in the same area of the brain", notes Mendonça. "Some neurons became active when the mouse was about to move, while others lit up when the mouse got its reward. But what really caught our attention was how these neurons reacted depending on which paw the mouse used".

How Dopamine Chooses Sides

The team noticed that the neurons excited by movement lit up more when the mouse used the paw opposite to the brain side being observed. For example, if they were looking at the right side of the brain, the neurons were more active when the mouse used its left paw, and vice versa. Digging deeper, the scientists found that the activity of these movement-related neurons not only signalled the start of a movement but also seemed to encode, or represent, the length of the movement sequences (the number of lever presses).

Mendonça elaborates, "The more the mouse was about to press the lever with the paw opposite the brain side we were observing, the more active

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neurons became. For example, neurons on the right side of the brain became more excited when the mouse used its left paw to press the lever more often. But when the mouse pressed the lever more with its right paw, these neurons didn't show the same increase in excitement. In other words, these neurons care not just about whether the mouse moves, but also about how much they move, and on which side of the body".

To study how losing dopamine affects movement, the researchers used a neurotoxin to selectively reduce dopamine-producing cells on one side of a mouse's brain. This method mimics conditions like PD, where dopamine levels drop and movement becomes difficult. By doing this, they could see how less dopamine changes the way mice press a lever with either paw. They discovered that reducing dopamine on one side led to fewer lever presses with the paw on the opposite side, while the paw on the same side remained unaffected. This provided further evidence for the side-specific influence of dopamine on movement.

Implications and Future Directions

Rui Costa, the study's senior author, picks up the story, "Our findings suggest that movement-related dopamine neurons do more than just provide general motivation to move - they can modulate the length of a sequence of movements in a contralateral limb, for example. In contrast, the activity of reward-related dopamine neurons is more universal, and doesn't favour one side over the other. This reveals a more complex role of dopamine neurons in movement than previously thought".

Costa reflects, "The different symptoms observed in PD patients could be perhaps related to which dopamine neurons are lost—for instance, those more linked to movement or to reward. This could potentially enhance management strategies in the disease that are more tailored to the type of dopamine neurons that are lost, especially now that we know there are different types of genetically defined dopamine neurons in the brain".

Technology Networks, 20 February 2024

https://yechnologynetworks.com

Solar-driven green synthesis of epoxides

2024-02-21

The review was led by Prof. Yuchao Zhang (Key Laboratory of Photochemistry, CAS Research/Education Center for Excellence in Molecular Sciences, Institute of Chemistry, Chinese Academy of Sciences)

Research published in the journal Science China Chemistry is expected to serve as comprehensive background knowledge and to provide researchers with insight into the recent developments of solar-driven green synthesis of epoxides.

"Epoxides play a pivotal role in industrial production, serving as essential building blocks or intermediates for synthesizing various high-value chemicals. Traditional preparation methods often rely on hazardous oxidants (such as peroxy acids) or extensive fossil fuel-powered thermal catalytic systems, resulting in significant CO2 emissions and waste production," Zhang says.

"Solar energy represents the most promising renewable energy source for a sustainable society. Recently, solar-driven photo(electro)chemistry has shown advantages in achieving the environmentally friendly synthesis of epoxides."

"For instance, hot electrons or local thermal effects generated on plasmonic photocatalysts can effectively lower the O2 activation temperature in the thermal catalysis system, and a photoelectrochemical system can efficiently reduce the applied voltage in the electrochemical halide-mediated indirect epoxidation process."

"However, there are still challenges that need to be addressed, including improving the efficiency of photo (electro)catalytic systems and gaining a deeper understanding of catalytic selectivity in epoxidation. A comprehensive review on this topic will provide further insights into this field and attract more researchers' attention to it."

In this review, the fundamental studies and reaction mechanisms of olefin epoxidation in three typical catalytic systems—molecular catalysis, heterogeneous thermal catalysis, and electrocatalysis—are summarized. Next, recent advances in utilizing solar energy to promote the synthesis of epoxides are discussed. Finally, insights into future perspectives on engineering photo(electro)chemical systems for efficient epoxide production are proposed.

Phys Org, 21 February 2024

https://phys.org

Tempering switches unique polymer from rigid cutlery to an adhesive to malleable plastic

2024-02-15

A plastic's properties are typically determined by chemical composition and, over the last century, scientists have developed hundreds of different polymers, each suited to a particular application. However, while some materials such as polyethylene can be remoulded, their fundamental characteristics such as hardness, brittleness and elasticity remain fixed, substantially limiting the uses of each polymer.

A single polymer feedstock has been used to form distinct plastic products including cutlery and adhesives – something that is impossible with conventional polymers.

Now, Stuart Rowan at the University of Chicago, US has developed a pluripotent polymer feedstock, enabling the team to alter the plastic's properties through careful control of the temperature just before it's ready to use. 'We were inspired by stem cells and their ability to differentiate into a range of different cell types in the human body, depending on environmental cues,' says Rowan. 'We made a polymer network that can be tempered, similar to the process in metals where a material is heated at a precise temperature before being rapidly cooled or quenched, [to] access materials that range from being hard and high strength to soft and extensible at room temperature.'

Conventional plastics cannot be tempered: thermoplastics such as polyethylene simply melt and thermoset plastics like epoxy resins decompose. However, the team designed a dynamic cross-linked polymer network in which the covalent bonds between the chemical components can reversibly break and form depending on the treatment temperature within the material's 'tempering window'. Between 60°C and 120°C this reversible bond reconfiguration allows the polymer to exhibit its unexpected 'pluripotency'. 'With different temperatures you can actually control the number of crosslinks,' explains Maarten Smulders, a dynamic polymers researcher from Wageningen University in the Netherlands who wasn't part of the new work. 'The higher the tempering temperature, the more bonds are opened up so there's a lower degree of adduct formation which results in a softer material.'

The quenching step halts this reversible bond breaking process and fixes properties in the material based on the extent of crosslinking. But the dynamic nature of these bonds means that the quenched plastic can also be re-tempered. 'You can reverse these changes and use the same material for different applications,' explains Filip Du Prez, a polymer chemist at Ghent University in Belgium. '[Rowan] has a very nice prototype – at 60°C he made a material that is good enough to work as a plastic fork or spoon. Then exactly the same material tempered at a higher temperature (110°C), he could use as an adhesive.'

Rowan's team is conscious that further development is needed to make the new plastic commercially viable. Slow heat dissipation through the polymer leads to long tempering times and the unusual chemical components are not readily available at scale. '[Another] next step is to improve the range of mechanical properties that our pluripotent materials

can access and to design pluripotent materials in which functional – as opposed to mechanical properties – can be tuned through tempering,' says Rowan.

But for Smulders and Du Prez, these early results offer a hugely exciting opportunity for polymer chemists, while also raising a number of intriguing questions. 'It's really interesting that they could maintain these properties at the quenched material's operating temperature,' comments Smulders. 'I would also love to learn more about the exact factors which produce this tempering window and drive the change in mechanical properties.'

'This has opened my eyes and might lead to a whole new generation of materials making use of dynamic chemistry,' says Du Prez. 'I'm thrilled to see what the future will bring and a big question for me is can we start to predict which other materials can show this property?'

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NR Boynton et al, Science, 2024, 383, 545 (DOI: 10.1126/science.adi5009)

Chemistry World, 15 February 2024

https://chemistryworld.com

Potential Alzheimer's Drug Discovered

2024-02-07

A potential new drug to prevent Alzheimer's disease in people with the so-called Alzheimer's gene has been discovered by a University of Arkansas for Medical Sciences (UAMS) research team led by Sue Griffin, Ph.D.

The findings were published Jan. 8 in Communications Biology and include discoveries of a druggable target and a drug candidate, made by Meenakshisundaram Balasubramaniam, Ph.D., the paper's first author.

An estimated 50-65% of people with Alzheimer's disease have inherited the Alzheimer's gene, Apolipoprotein E4 (APOEε4), from one or both parents. About 25% of people have one copy of APOEε4 and are three times as likely to develop the disease. Those with two copies (one from each parent) make up 2-3% of the population and are 12-15 times as likely to develop Alzheimer's.

Griffin said her team appears to be the first with the new drug-related discoveries just as it was first in 2018 to show how APOEε4 prevented

An estimated 50-65% of people with Alzheimer's disease have inherited the Alzheimer's gene.

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brain cells from disposing of their waste products, known as lysosomal autophagy.

Such disruption of autophagy in those who inherit APOEε4 is responsible for the formation of plaques and tangles in the brain that are hallmarks of Alzheimer's disease. That groundbreaking discovery was published in Alzheimer's and Dementia, the Journal of the Alzheimer's Association.

"Our series of discoveries related to APOEε4 and its detrimental role in Alzheimer's pathogenesis are among the most impactful of my 50 years as a research scientist," said Griffin, a pioneer in the study of neuroinflammation and co-founder of the Journal of Neuroinflammation, based at the UAMS Donald W. Reynolds Institute on Aging. "No other research team has found a potential drug specifically for blocking the harmful effects of inherited APOEε4."

Griffin is the Alexa and William T. Dillard Chair in Geriatric Research and a distinguished faculty scholar in the College of Medicine and director of research at the Institute on Aging. She is also a professor in the college's departments of Neurobiology & Developmental Sciences, Internal Medicine and Psychiatry. Notably, she is a winner of the Alzheimer's Association's Lifetime Achievement Award and inductee of the Arkansas Women's Hall of Fame.

Most Alzheimer's research nationally has focused on treatments that can clear away the brain's plaques and tangles associated with the disease, but that approach has yielded unimpressive results. Griffin notes that people with mild Alzheimer's symptoms have already lost about half or more of the neurons responsible for memory and reasoning, which has led to her focus on prevention.

Griffin's team is advancing its innovative work with a recent five-year, $2.35 million grant from the National Institutes of Health (NIH). The team will conduct larger-scale preclinical research on the drug candidate, CBA2, as well as test other potential drug candidates.

"Our hope is that people who have one or two copies of APOEε4 will one day take the drug regularly throughout their life and significantly reduce their risk of developing Alzheimer's disease," Griffin said.

Balasubramaniam, co-principal investigator on the NIH grant with Griffin, said UAMS built the first known full-length structure of APOEε4 protein in 2017, which he created using bioinformatics and computational modeling techniques. This foundational work led to the discovery of the druggable

site on the APOEε4 protein, ApoE4. (APOEε4 refers to the gene, and ApoE4, without the epsilon symbol and no italics, is the protein.)

Balasubramaniam's unique skills and curiosity, Griffin said, were the catalyst for the discoveries.

"I don't know of anyone else in the world but Dr. Balasubramaniam who can do the work that's in this paper," Griffin said of the assistant professor and Inglewood Scholar in the Department of Geriatrics.

While most institutions still manually screen drug compounds, which can take years, Balasubramaniam oversees a computational biology suite with high-performance GPU servers that he used to screen about 800,000 compounds in two days.

His computer-simulated findings on ApoE4-targeted drug actions were validated in various in vitro and in vivo model systems.

Technology Networks, 07 February 2024

https://technologynetworks.com

Pharmacists propose ways to increase the activity of levofloxacin and overcome bacterial resistance

2024-02-21

Generation refers to different modifications of quinolones that are used in different areas. Quinolones of different generations are widely used, but bacteria—for example, pneumococcus and Staphylococcus aureus—develop resistance to them. RUDN University pharmacists studied several derivatives of levofloxacin to find potential candidates for new antibacterial drugs and find out which structural elements are responsible for the biological activity of the substances.

"One of the approaches to improve the kinetic and dynamic characteristics of drugs is to study the properties of the products that are formed as a result of their transformation," Elena Uspenskaya, Doctor of Pharmaceutical Sciences, Professor, Associate Professor of the Department of Pharmaceutical and Toxicological Chemistry of the RUDN University said.

For the experiment, scientists used the pharmaceutical substance levofloxacin. To predict what biological activity its derivatives will have, the authors simulated them, as well as molecular docking "poses" on a computer (in silico). A total of five derivatives and levofloxacin itself were studied. Biological activity was assessed using 7 different types of activity:

The antibacterial drug levofloxacin is used to treat pneumonia, sinusitis, genitourinary infections, and other diseases. It is included in the WHO Model List of Essential Medicines.

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antibacterial and antitumor effects, inhibition of specific enzymes, and so on.

Modeling made it possible to determine which structural elements of levofloxacin are responsible for its action. Thus, without a carboxyl group in the composition, the antimicrobial activity of the substance is reduced by half. Non-standard actions appear—for example, suppression of the cytochrome P450 enzyme. For some of the most promising modifications, the authors obtained 3D renderings. Based on these results, it will be possible to search for new drugs based on levofloxacin.

"The in silico results allowed us to discover quantitative structure-activity correlations and predict the molecular mechanisms of activity. This is of applied interest for targeted drug search," Elena Uspenskaya, Doctor of Pharmaceutical Sciences, Professor, Associate Professor of the Department of Pharmaceutical and Toxicological Chemistry of the RUDN University said.

The study is published in the journal Scientia Pharmaceutica.

Phys Org, 21 February 2024

https://phys.org

Advanced artificial photosynthesis catalyst uses CO2 more efficiently to create biodegradable plastics

2024-02-16

Amid growing global concern over climate change and plastic pollution, researchers at Osaka Metropolitan University are making great strides in the sustainable production of fumaric acid -- a component of biodegradable plastics such as polybutylene succinate, which is commonly used for food packaging.

The researchers have managed to efficiently produce fumaric acid, which is traditionally derived from petroleum, using renewable resources, carbon dioxide, and biomass-derived compounds.

In a previous study, a research team led by Professor Yutaka Amao of the Research Center for Artificial Photosynthesis at Osaka Metropolitan University demonstrated the synthesis of fumaric acid from bicarbonate and pyruvic acid, a biomass-derived compound, using solar energy.

They also succeeded in producing fumaric acid using carbon dioxide obtained directly from the gas phase as a raw material.

A research team from Osaka Metropolitan University that had previously succeeded in synthesizing fumaric acid using bicarbonate and pyruvic acid, and carbon dioxide collected directly from the gas phase as one of the raw materials, has now created a new photosensitizer and developed a new artificial photosynthesis technology, effectively doubling the yield of fumaric acid production compared to the previous method.

However, the yield in the production of fumaric acid remained low.

In their latest research, published in Dalton Transactions, the researchers have now developed a new photosensitizer and further advanced an artificial photosynthesis technique that doubles the yield of fumaric acid compared to conventional methods.

"This is an extremely important advancement for the complex bio/photocatalyst system. It is a valuable step forward in our quest to synthesize fumaric acid from renewable energy sources with even higher yields, steering us toward a more sustainable future," said Professor Amao.

Science Daily, 16 February 2024

https://sciencedaily.com

Super-thickeners made from starch reduce calories and carbs in food

2024-02-16

Building tiny sheets and cages from starch particles turns them into super-thickeners that could reduce the calorie content of foods.

Starch is often added to foods like soups to make them richer and thicker, but doing so increases the calorie count and carbohydrate content. Now, Peilong Li at Cornell University in New York and his colleagues have found that the amount of starch in foods can be reduced without sacrificing texture by arranging starch particles into special shapes.

Starch particles thicken food because they swell up when they are heated. This means the particles jam against each other, leaving less room for liquid components of the dish to flow freely. The researchers wondered whether they could replicate this effect but cut the amount needed by hollowing out globs of starch. "But you can't just carve a starch granule like it's a pumpkin," says Li.

Instead, working with starch particles extracted from amaranth grain, he and his colleagues devised a way to assemble them into three-dimensional shapes by mixing them with water and oil. The starch particles arranged themselves around oil drops, and then the researchers removed the two liquids through a combination of heating and freeze-drying. This left them with just the starchy structures, some shaped like cages with hollow centres, some shaped like sheets that would cascade on top of each other so liquids would get trapped between them.

Assembling starch granules into 3D shapes could achieve the same thickening effect in foods with up to 50 per cent fewer granules, reducing the calories and carbohydrates without sacrificing texture

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The team discovered that these starch structures performed so well as thickening agents that they could be used to halve the amount of starch typically needed to thicken foods.

Fan Zhu at the University of Auckland in New Zealand says that using these granules as building blocks for the new class of hollow starch structures is very innovative and could make starches a big part of designing future foods. However, Zhu says that amaranth starch is expensive and can be difficult to source in large quantities, so adapting the new method to more affordable and abundant starches like those made from corn would be advantageous. "And more studies are needed on what happens when you put this kind of structure in your mouth," he says.

New Scientist, 16 February 2024

https://newscientist.com

Researchers synthesize a new manganese-fluorine catalyst with exceptional oxidizing power

2024-02-20

Led by Professor Jaeheung Cho in the Department of Chemistry at UNIST, the research team successfully synthesized the pioneering manganese-fluorine catalyst, utilizing the Macrocyclic Pyridinophane System. This catalyst demonstrates the ability to induce oxidation reactions, facilitating efficient electron loss from toxic toluene derivatives. The work is published in the Journal of the American Chemical Society.

Through meticulous analysis, the research team has uncovered the underlying mechanisms responsible for the catalyst's exceptional performance in oxidation reactions. By modulating the electronic environment of various compounds, the team verified the catalyst's capability to catalyze the oxidation of toluene derivatives with unparalleled efficiency.

This research represents the first exploration of the physicochemical properties of transition metal-fluorine species, introducing a new paradigm for carbon-hydrogen bond decomposition based on electron transfer reactions.

Professor Cho emphasized the significance of activating organic matter with robust carbon-hydrogen bonds, highlighting their propensity to accept electrons and undergo reduction through high reduction potential

A research team, affiliated with UNIST has unveiled a cutting-edge catalyst with exceptional oxidizing power, capable of extracting electrons from compounds.

chemical reactions. The unique characteristics of manganese-fluorine species enable catalytic transformations in this context.

The advancement of organic catalysts through carbon-hydrogen (C-H) bond activation is a crucial research area with extensive applications in pharmaceuticals and industrial processes. Efforts are underway to develop cost-effective metal catalysts by emulating the activities of diverse metal enzymes through bio-simulation research.

Recent focus has been directed towards metal-halide materials that combine transition metals like iron and manganese with halogen atoms, particularly fluorine, acting as intermediates for oxidizing diverse organic substances. The newly synthesized manganese-fluorine catalyst emerges as the most reactive metal-halide species disclosed to date, offering promising applications in industrial processes.

The research team analyzed the oxidation mechanism facilitated by the catalyst, showcasing enhanced reaction rates by manipulating the electronic environment of various compounds. The catalyst's remarkable efficiency in oxidizing toluene derivatives, a feat previously unseen with existing metal-halide species, is also noteworthy.

The study was co-authored by researchers Donghyun Jeong and Yujeong Lee under the guidance of Professor Cho. The research not only propels carbon-neutral technologies forward but also contributes to the advancement of next-generation academics and pivotal progress in environmental and industrial sectors.

Phys Org, 20 February 2024

https://phys.org

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CHEMICAL EFFECTS

ENVIRONMENTAL RESEARCH

PHARMACEUTICAL/TOXICOLOGY

OCCUPATIONAL