CHEMWATCH

Bulletin Board

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CURIOSITIES

TECHNICAL NOTES

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ASIA PACIFIC

'odd-even rule not suitable for delhi'

2023-11-12

Before Diwali celebrations even began, Delhi's AQI index hit the "severe" level. Anticipating a worsening situation, the Delhi administration, five days after implementing GRAP-4, had decided to impose an odd-even scheme, but after two days of rain in the national capital, Environment Minister Gopal Rai said that the odd-even car rationing scheme will not be implemented from 13-20 November as there has been a significant improvement in Delhi's air quality.

After the initial announcement of implementation of the odd-even rule, Delhi residents had feared that the move would trigger traffic chaos in the national capital. Here are five reasons why without proper planning, the odd-even scheme can't be successful in the national capital.

Capacity of Public Transportation

An effective public transport system is necessary for the odd-even rule to work properly in order to handle the additional demand on days when half of the automobiles are limited. Though there is good metro connectivity in Delhi, it's still overloaded in many routes, including the blue and yellow lines. So, in places like Delhi, the infrastructure for public transport might not be able to support the extra traffic, and commuters may have trouble locating other options.

A resident of Gurugram, Dakshesh Kashyap, said: "When it was announced that the scheme would be implemented, it made me tense thinking about the struggle in the metro, price hikes by auto, uber, and even local auto drivers. People like us have to travel from Gurugram to Delhi, which approximately takes two hours of travel on our own vehicle, but it may take 2:30-3 hours if the odd-even plan is implemented. So, my entire timetable will get disturbed, and since the rule will be for all, there will be a crowd on the buses as well."

Read More

The Sunday Guardian, 12-11-23

https://sundayguardianlive.com/news/odd-even-rule-not-suitable-for-delhi

The ambient air quality standards, green innovation, and urban air quality: evidence from China

2023-11-11

As China's economy transitions, environmental issues have become a major concern. This study examines the impact of Ambient Air Quality Standards (AAQS) on urban air quality using panel data from 284 cities in China from 2006 to 2019. The study utilizes DID (Difference-in-Difference) models to analyze the regulatory effects of AAQS and its spatial spillover. Additionally, the serial multiple mediation models are constructed to investigate the role of green innovation. The findings reveal that the AAQS positively affects urban air quality, albeit with a notable "hysteresis effect." Local implementation of AAQS worsens air quality in neighboring cities within a distance of 400 km, but beyond 400 km, the effect is reversed. Heterogeneity analysis shows that AAQS improves air quality in central cities, large-sized and medium-sized cities, cities with weak environmental governance, and resource-based cities. Mechanism tests suggest that AAQS may enhance urban air quality by promoting green innovation and optimizing industrial structure. Especially, either the energy-use effect or industrial-structure effect triggered by green innovation can contribute to the improvement of urban air quality.

Introduction

Managing the balance between environmental protection and economic development is crucial for achieving sustainable development in China. The economic growth resulting from reform and opening up has propelled China to become the world`s second-largest economy. However, this rapid development has also brought about significant challenges, particularly in terms of ecological imbalance and environmental pollution, especially air pollution. Despite some improvements, the governance efforts have not met expectations. According to the 2020 China Ecological Environment Status Bulletin, approximately 40.1% of the cities at the prefecture-level and above still fail to meet the "Ambient Air Quality Standards" (National standard number: GB 3095-2012) implemented in 2012. Urban air pollution remains a persistent issue, especially during unfavorable weather conditions when severe air pollution occurrences are frequent.

Read More

Scientific Reports, 11-11-23

https://www.nature.com/articles/s41598-023-47112-w

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Overview of Hazchem QR Code Application in China

2023-11-16

China's "One Enterprise, One Product, One QR Code" policy for hazardous chemical management has gained significant attention in the global supply chain. In this article, ChemLinked will navigate you through the development and requirements regarding Hazchem management based on QR codes.

The use of quick response (QR) codes, a type of barcode that stores information and can be easily read by digital devices, has become prevalent in tracking product information in the supply chain. Recognizing the convenience of this technique, the Ministry of Emergency Management (MEM) of China introduced the "One enterprise, One product, One QR code" policy to enhance the digital and intelligent management of hazardous chemicals (Hazchem). This policy was introduced in the National Plan for Centralized Management of Safety Risks of Hazardous Chemicals issued in January 2022.

The pilot project for the Hazchem QR code application commenced in Guangdong, a province designated by the State, in June 2021. Since October 2021, the Hazchem QR code has been mandatory on hazardous chemical labels, packaging, containers and vehicles before hazardous chemicals leave the factory or warehouse in Guangdong. On January 29, 2022, Guangdong issued its Local Plan for Centralized Management of Safety Risks of Hazardous Chemicals, fully implementing the "One enterprise, One product, One QR code" policy in the province.

Drawing from Guangdong's experience, the MEM launched in February 2022 the new online platform - Hazardous Chemical Registration Comprehensive Service System to support the automatic generation of QR codes for registered hazardous chemicals nationwide. Several other provinces and cities in China, e.g., Shandong, Jiangsu, Zhejiang, Shanghai, etc., have also initiated relevant plans or pilot projects to push forward the Hazchem QR code application (see the map below). Details can be accessed here.

Currently, pilot provinces and cities are studying their own pilot projects based on local conditions to push forward the "One enterprise, One product, One QR code" policy. At the national level, the policy has not yet been fully implemented so far.

The major requirements for the Hazchem QR code application are as follows.

Read More

Chemlinked, 16-11-23

https://chemical.chemlinked.com/expert-article/overview-of-hazchem-qr-code-application-in-china

New Zealand Consults on Cutting Lead Levels in Paints

2023-11-13

The lead level limit for paint will be lowered to 0.009% (90ppm), in line with countries including Australia, Canada and the United States.

The Environmental Protection Authority (EPA) of New Zealand is calling for submissions regarding proposed changes to a series of group standards to reduce the maximum allowable levels of lead in paint.

Interested parties are encouraged to provide information, make comments, and raise issues to contribute to the EPA decision-making process. The deadline for submissions is January 26, 2024.

Group standards are approvals and rules for using a group of hazardous substances of a similar nature, type or use. The following group standards are currently in place for the management of paints in New Zealand:

- Surface Coatings and Colourants Group Standards: covering most paints
- Aerosols Group Standards: covering spray paints
- Corrosion Inhibitors Group Standards: covering anti-rust paints and products
- Graphic Materials Group Standard: covering painting and drawing products

The current lead level limit for paints covered by the Surface Coatings and Colourants Group Standards and the Aerosols Group Standards is 0.1% (1000 parts per million/ppm). The proposed changes seek to reduce this limit to 0.009% (90ppm), aligning with countries such as Australia, Canada and the United States.

The Corrosion Inhibitors Group Standards currently do not specify any maximum lead level limits. The EPA proposes amending the group standards to include lead level limits in the same way as the Surface Coatings and Colourants Group Standards and the Aerosols Group Standards.

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Chemlinked, 13-11-23

https://chemical.chemlinked.com/news/chemical-news/new-zealand-consults-on-cutting-lead-levels-in-paints

Singapore publishes new regulations to offset carbon tax by carbon credits

2023-11-16

The following three regulations related to the Carbon Pricing Act were promulgated in Singapore on October 6, 2023. All of the regulations will take effect on January 1, 2024(*). In Singapore, under the Carbon Pricing (Amendment) Act 2022 promulgated on March 7, 2023, in addition to the "fixed-price carbon credit" (FPCC), eligible international carbon credits (ICC) that meet the prescribed criteria will be available for carbon tax payments. The three regulations specify the criteria for eligible international carbon credits, its application and its surrender.

- Carbon Pricing (Measurement, Reporting and Verification) (Amendment) Regulations 2023

https://sso.agc.gov.sg/SL-Supp/S659-2023/Published/20231006?DocDate=20231006&ViewType=Pdf&_=20231006184301

- Carbon Pricing (Registration and General Matters) (Amendment) Regulations 2023

https://sso.agc.gov.sg/SL-Supp/S660-2023/Published/20231006?DocDate=20231006&ViewType=Pdf&_=20231006184301

- Carbon Pricing (Carbon Tax and Carbon Credits Registry) (Amendment) Regulations 2023

https://sso.agc.gov.sg/SL-Supp/S661-2023/Published/20231006?DocDate=20231006&ViewType=Pdf&_=20231006184301

(*) Article 8 of the Carbon Pricing (Registration and General Matters) (Amendment) Regulations 2023 shall be deemed to have come into force on December 31, 2021. This Article 8 changes part of the name of the cited law (Evidence Act 1893) and is not a provision related to the carbon pricing regulations.

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Envilliance, 16-11-23

https://enviliance.com/regions/southeast-asia/sg/report_11140

AMERICA

Why Is The Air Force Removing AFFF from It's Hangar Fire Safety Systems?

2023-11-12

Read more: https://programminginsider.com/why-is-the-air-force-removing-afff-from-its-hangar-fire-safety-systems/

Aqueous Film Forming Foam, or AFFF, represents a significant advancement in firefighting technology, particularly within the high-stakes environment of military operations. Originally developed in the 1960s, AFFF has been instrumental in quickly extinguishing intense fuel-based fires. AFFF creates a blanket that starves the fire of oxygen while simultaneously cooling the fuel surfaces. This has made it the go-to option for hangar fire suppression in the U.S. Air Force for decades.

The U.S. Air Force's decision to phase out AFFF did not come lightly. It emerged from an accumulation of scientific research, environmental considerations, and an evolving understanding of the long-term impact of firefighting foam usage. Let's explore further. Regulatory and Policy Shifts The landscape of environmental regulation and safety protocols has been undergoing significant changes with regard to AFFF. Despite its efficacy, the substance fell under this scrutiny due to the persistent nature of its key components: perfluoroalkyl and polyfluoroalkyl substances (PFAS). These compounds have been linked to environmental degradation and health issues, catalyzing a reexamination of their widespread use. In the United States, environmental regulations have tightened as scientific understanding of the impacts of PFAS has grown. The Environmental Protection Agency (EPA), alongside other federal agencies, has released advisories and is moving toward setting enforceable limits for PFAS in the environment. This shift in policy comes after decades of PFAS compounds accumulating in the environment, largely unchecked due to the lack of comprehensive regulation historically.

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Programming Insider, 12-11-23

https://programminginsider.com/why-is-the-air-force-removing-afff-from-its-hangar-fire-safety-systems/

EUROPE

Calls for Information on Persistent Organic Pollutants

2023-11-13

The Department for Environment, Food and Rural Affairs (Defra) are inviting stakeholders to provide information regarding a number of proposed POPs ahead of a meeting of the POPs Review Committee (POPRC).

The UK is a party to the Stockholm Convention on POPs, which are substances that persist in the environment, accumulate in living organisms, pose a risk to our health and the environment, and have the potential for long range transport across international borders.

Additional information is requested for the following substances:

Chlorpyrifos

This is an insecticide which is no longer registered for use in the UK.

The requested information relates to socio-economic considerations to assist the drafting of a Risk Management Evaluation (as specified in Annex F of the Stockholm Convention).

Further details and information submission forms for chlorpyrifos can be found on GOV.UK.

Completed forms and/or queries should be directed to the Defra POPs team atPOPs@defra.gov.uk

Deadline: 24 November 2023

Medium chain chlorinated paraffins (MCCPs)

Industrial chemical. Newly recommended for listing as a POP under the Stockholm Convention.

In October 2023, POPRC agreed the Risk Management Evaluation for MCCPs, and decided to recommend to the Conference of Parties (COP)

2025, that it considers listing MCCPs for elimination (under Annex A of the Stockholm Convention) with specific exemptions for several applications.

The Committee have invited Parties and observers to provide information that would assist in the possible strengthening of the recommendations by the Committee.

Further details and information submission forms for MCCPs can be found on the POPRC call for information.

Deadline: 18 January 2024

Long-chain perfluorocarboxylic acids (LC-PFCAs)

Industrial chemical. Newly recommended for listing as a POP under the Stockholm Convention.

POPRC has agreed the Risk Management Evaluation of LC-PFCAs, their salts, and related compounds, and the substance is recommended to the COP 2025 to be listed for elimination (under Annex A of the Stockholm Convention).

The Committee have invited Parties and observers to provide information that would assist in the possible refining of recommended specific exemptions for production and use of LC-PFCAs.

Further details and information submission forms for LC-PFCAs can be found on the POPRC call for information.

Deadline: 18 January 2024

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HSE.UK, 13-11-23

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

EU Plans Legislation to Reduce Methane Emissions from Fossil Fuels

2023-11-16

The EU Commission has reached a provisional agreement for a new regulation aimed at reducing methane emissions from fossil fuels in the European energy sector and international supply chains.

The regulation would include required measuring, monitoring, and reporting of methane emissions from the gas, oil, and coal industries and

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plans to enforce action towards making necessary emissions reductions. The EU aims for methane abatement to contribute greatly to the European Green Deal goal of lowering emissions by at least 55% by 2030.

The Commission said it is the first law in the EU to tackle methane emissions.

Specifics from the proposed EU Regulation include a number of rules for reporting methane emissions and providing transparent updates on reduction activities. This includes regular surveys of equipment to check for methane leaks, bans of routine venting and flaring, and limited venting from thermal coal mines, among others.

Since the EU imports much of the fossil fuel energy sources it consumes, the regulations will also address methane emissions from these supply chains. The regulation agreement includes the establishment of a methane transparency database, global methane emitters monitoring tools, and monitoring obligations for new import contracts of oil, gas, and coal starting in 2027.

Read More

Environment + Energy Leader, 16-11-23

https://www.environmentenergyleader.com/2023/11/eu-plans-legislation-to-reduce-methane-emissions-from-fossil-fuels/

INTERNATIONAL

'New asbestos' warning to chemical sector from investors with $10 trillion in assets

2023-11-15

PRESS RELEASE: PFAS chemicals are 'the new asbestos' for the chemical sector and firms should follow 3M's lead and quit production, a group of over 50 institutional investors and their representatives warned today.

Published on 15 Nov 2023

Read this story in today's Financial Times.

***

The Investor Initiative on Hazardous Chemicals (IIHC), which represents over $10 trillion in assets under management or advice, wrote to the

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CEOs of the world's 50 largest stock-listed chemical companies saying: "Manufacturers and users of PFAS chemicals are exposed to deep liability and insurance risks, reminiscent of those historically linked to asbestos, which could materially adversely harm the long-term value of companies involved in their manufacture and sale." Production and use should be phased out, it said. Parts of the letter were published by IIHC coordinator, the International Chemical Secretariat (ChemSec).

IIHC collectively represents over $10 trillion in assets under management or advice and includes Storebrand Asset Management, Allianz Investment Management, BNP Paribas Asset Management and Resona Asset Management. Members stepped up their interventions this year, holding meetings with 16 chemical firms on production reforms, a level of pressure from institutional investors the sector has not seen before.

For decades, asbestos was known as the magic mineral, despite early health concerns that eventually led to lawsuits and numerous bankruptcies that continue to this day. PFAS hazards were also recognised early, but production today is at an all-time high. US companies face a flood of lawsuits, with defendants expanding beyond producers to PFAS users in the auto, food, textiles, cosmetics and paper sectors. The first bankruptcy occurred this year and more are expected, experts told Bloomberg. In Europe, 3M reached a €500m settlement last year, but fresh lawsuits have begun in the Netherlands and Belgium. Both US states and the European Union are drafting PFAS bans.

Read More

Chemsec, 15-11-23

https://chemsec.org/new-asbestos-warning-to-chemical-sector-from-investors-with-10-trillion-in-assets/

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REACH Update

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ECHA identifies research needs for regulating hazardous chemicals

2023-11-15

The European Chemicals Agency (ECHA) has published a new report on 'Key areas of regulatory challenge 2023' that identifies areas where research is needed to protect people and the environment from hazardous chemicals. It also highlights where new methods, that support the shift away from animal testing, are needed.

Helsinki, 15 November 2023 – To further improve chemical safety in the EU, scientific research needs to deliver data that is relevant to regulating chemicals. In order to enhance the regulatory relevance of scientific data, ECHA has identified the following areas as priorities for research.

- Hazard identification for critical biological effects that currently lack specific and sensitive test methods: i.e. developmental and adult neurotoxicity, immunotoxicity and endocrine disruption
- Chemical pollution in the natural environment (bioaccumulation, impact on biodiversity, exposure assessment);
- Shift away from animal testing (read across under REACH, move away from fish testing, mechanistic support to toxicology studies e.g. carcinogenicity)
- New information on chemicals (polymers, nanomaterials, analytical methods in support of enforcement)

Mike Rasenberg, ECHA Director of Hazard Assessment says:"ECHA believes that to achieve the ambitions of the European Green Deal and the EU's Chemicals Strategy for Sustainability we need more scientific research with regulatory relevance.

"There is a growing need for new test methods that do not rely on animals, and a better understanding of the toxicological mode of action of certain hazardous chemicals. Generating the necessary data without animal testing while protecting health and the environment, cannot be achieved without scientific progress. "We encourage the scientific community to take this opportunity and work with us to contribute to a safer Europe."

Read More
ECHA, 15-11-23

https://echa.europa.eu/-/echa-identifies-research-needs-for-regulating-hazardous-chemicals

Oxygen and Nitrogen

2023-11-24

https://www.periodictable.co.za/blog/chemistry-jokes

Carbaryl

2023-11-24

USES [2,3]

Carbaryl is commonly sold under the trade name Sevin, and goes by trade names such as Adios, Carbamec, Denapon, Hexavin, and Panam. Its primary use is as an insecticide on various commercial crops, including but not limited to corn, soybean, cotton, citruses, pears, and nuts. In addition to also being effective as a molluscicide and acaricide, carbaryl can also be used to treat pest infestations, such as that due to species of lice, on livestock, poultry, pets, and in the case of head lice, on people.

EXPOSURE SOURCES & ROUTES OF EXPOSURE [3]

Exposure Sources

- Individuals are most likely to be exposed to carbaryl dermally or by inhalation during the manufacture, formulation, and application of this pesticide.
- The general public may be exposed to carbaryl from spray drift in regions surrounding agricultural areas.
- Carbaryl has been detected at low levels in surface water and in food.

Routes of Exposure

The main exposure routes for carbaryl are:

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

HEALTH EFFECTS [4]

Acute Health Effects

- Acute occupational exposure of humans to carbaryl has been observed to cause cholinesterase inhibition (which impairs central nervous system (CNS) function), resulting in nausea, vomiting, bronchoconstriction, blurred vision, convulsions, coma, and respiratory failure.

Carbaryl is the common name for a chemical known as 1-naphthyl methylcarbamate. Carbaryl is a white crystalline solid that is slightly soluble in water. It is essentially odourless and its odour threshold has not been established.

- Acute carbaryl exposure in humans may also cause eye and skin irritation.
- Tests involving acute exposure of rats, mice, rabbits, and guinea pigs have demonstrated carbaryl to have moderate to high acute toxicity from ingestion and moderate acute toxicity from dermal exposure.

Carcinogenicity

- No information is available on the carcinogenic effects of carbaryl in humans.
- No significant increase in tumour incidence was found among exposed animals in several studies.
- EPA has not classified carbaryl for carcinogenicity.

Other Effects

- No information is available on the reproductive or developmental effects of carbaryl in humans.
- Two studies produced teratogenic effects in dogs fed carbaryl, but dogs were judged inappropriate for human health risk assessment because of differences in metabolism. Other studies demonstrating teratogenic effects also caused maternal toxicity.
- Reduced fertility and litter size and increased mortality in offspring have been observed in rats exposed to carbaryl in their diet over three generations.

SAFETY

First Aid Measures [5]

- Swallowed: If poisoning occurs, contact a doctor or Poisons Information Centre (ph: 13 11 26).
- Eye: Immediately irrigate with copious quantities of water for at least 15 minutes. Seek medical assistance.
- Skin: If material is splashed onto the skin, remove any contaminated clothing and wash skin thoroughly with water and soap if available and give one atropine tablet every 5 minutes until dryness of the mouth occurs. Urgently transport to hospital or doctor.
- Inhaled: Remove victim to fresh air. Apply resuscitation if victim is not breathing - DO NOT use direct mouth-to-mouth method if victim ingested or inhaled substance; use alternative respiratory method or proper respiratory device - Administer oxygen if breathing is difficult.

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- Give on atropine tablet every 5 minutes until dryness of the mouth occurs. Seek immediate medical assistance.

First Aid Facilities:

- Eye wash fountain;
- Safety shower and normal wash room facilities.

Workplace Controls & Practices [4]

Engineering Controls

- Carbaryl is a toxic material and a single significant exposure may cause death.
- Maintain adequate ventilation at all times.
- Prevent accumulation of gas(es) in hollows or sumps.
- Eliminate any sources of ignition.
- DO NOT enter room unless monitored by another person (ie buddy-buddy system).
- Sampling of the atmosphere if possible should be conducted automatically instead of human operator and any leaks discovered should then be directed digitally to a command centre where the event can be acted upon, with all appropriate procedures being implemented and including any protective equipment as outlined in this MSDS.

Personal Protective Equipment [5]

the following personal protective equipment is recommended when handling carbaryl:

- **CLOTHING:** PVC, Nitrile, Neoprene, Natural rubber or any other type of apron or splash suit as recommended by the manufacturer.
- **GLOVES:** PVC, Nitrile, Neoprene, Natural rubber or any other type of glove as recommended by the manufacturer.
- **EYES:** Chemical goggles or face shield to protect eyes.
- **RESPIRATORY PROTECTION:** Avoid breathing of gases. Select and use respirators in accordance with AS/NZS 1715/1716. When gases exceed the exposure standards then the use of an atmosphere-supplied, positive pressure demand self-contained or airline breathing apparatus supplied air respirator complying with the requirements of AS/NZS 1715 is recommended. Filter capacity and respirator type depends on exposure levels.

- If entering spaces where the airborne concentration of a contaminant is unknown then the use of a self-contained breathing apparatus (SCBA) with positive pressure air supply complying with AS/NZS 1715 / 1716, or any other acceptable International Standard is recommended.

REGULATION

United States

NIOSH: The National Institute of Occupational Safety & Health has set a Relative Exposure Limit (REL) for carbaryl of TWA 5 mg/m3.

OSHA: The Occupational Safety & Health Administration has set a Permissible Exposure Limit (PEL) for carbaryl of TWA 5 mg/m3.

ACGIH: The American Conference of Governmental Industrial Hygienists has set a Threshold Limit Value (TLV) for carbaryl of TWA 5 mg/m3.

Australia

Safe Work Australia: Safe Work Australia has set a Time Weighted Average (TWA) concentration for an 8-hour workday of 5 mg/m3 for carbaryl.

REFERENCES

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How is decaf coffee made? And is it really caffeine-free?

2023-11-01

However, some people prefer to limit their caffeine intake for health or other reasons. Decaffeinated or "decaf" coffee is widely available, and its consumption is reported to be on the rise.

Here's what you need to know about decaf coffee: how it's made, the flavour, the benefits – and whether it's actually caffeine-free.

How is decaf made?

Removing caffeine while keeping a coffee bean's aroma and flavour intact isn't a simple task. Decaf coffee is made by stripping green, unroasted coffee beans of their caffeine content and relies on the fact that caffeine dissolves in water.

Three main methods are used for removing caffeine: chemical solvents, liquid carbon dioxide (CO_2), or plain water with special filters.

The additional steps required in all of these processing methods are why decaf coffee is often more expensive.

Solvent-based methods

Most decaf coffee is made using solvent-based methods as it's the cheapest process. This method breaks down into two further types: direct and indirect.

The direct method involves steaming the coffee beans and then repeatedly soaking them in a chemical solvent (usually methylene chloride or ethyl acetate) which binds to the caffeine and extracts it from the beans.

After a pre-determined time, the caffeine has been extracted and the coffee beans are steamed once more to remove any residual chemical solvent.

The indirect method still uses a chemical solvent, but it doesn't come into direct contact with the coffee beans. Instead, the beans are soaked in hot water, then the water is separated from the beans and treated with the chemical solvent.

The caffeine bonds to the solvent in the water and is evaporated. The caffeine-free water is then returned to the beans to reabsorb the coffee flavours and aromas.

Coffee is one of the most popular drinks in the world, and its high levels of caffeine are among the main reasons why. It's a natural stimulant that provides an energy buzz, and we just can't get enough.

The solvent chemicals (particularly methylene chloride) used in these processes are a source of controversy around decaf coffee. This is because methylene chloride is suggested to be mildly carcinogenic in high doses. Methylene chloride and ethyl acetate are commonly used in paint stripper, nail polish removers and degreaser.

However, both the Australian New Zealand Food Standards Code and the United States Food and Drug Administration permit the use of these solvents to process decaf. They also have strict limits on the amount of the chemicals that can still be present on the beans, and in reality practically no solvent is left behind.

Non-solvent-based methods

Non-solvent-based methods that use liquid carbon dioxide or water are becoming increasingly popular as they don't involve chemical solvents.

In the CO_2 method, liquid carbon dioxide is pumped into a high-pressure chamber with the beans, where it binds to the caffeine and is then removed through high pressure, leaving behind decaffeinated beans.

The water method (also known as the Swiss water process) is exactly what it sounds like – it involves extracting caffeine from coffee beans using water. There are variations on this method, but the basic steps are as follows.

For an initial batch, green coffee beans are soaked in hot water, creating an extract rich in caffeine and flavour compounds (the flavourless beans are then discarded). This green coffee extract is passed through activated charcoal filters, which trap the caffeine molecules while allowing the flavours to pass through.

Once created in this way, the caffeine-free extract can be used to soak a new batch of green coffee beans – since the flavours are already saturating the extract, the only thing that will be dissolved from the beans is the caffeine.

Is caffeine fully removed from decaf?

Switching to decaf may not be as caffeine free as you think.

It is unlikely that 100% of the caffeine will be successfully stripped from the coffee beans. Just like the caffeine content of coffee can vary, some small amounts of caffeine are still present in decaf.

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However, the amount is quite modest. You would need to drink more than ten cups of decaf to reach the caffeine level typically present in one cup of caffeinated coffee.

Australia does not require coffee roasters or producers to detail the process used to create their decaf coffee. However, you might find this information on some producers' websites if they have chosen to advertise it.

Does decaf coffee taste different?

Some people say decaf tastes different. Depending on how the beans are decaffeinated, some aromatic elements may be co-extracted with the caffeine during the process.

Caffeine also contributes to the bitterness of coffee, so when the caffeine is removed, so is some of the bitterness.

Do caffeinated and decaf coffee have the same health benefits?

The health benefits found for drinking decaf coffee are similar to that of caffeinated coffee, including a lower risk of type 2 diabetes, some cancers and overall mortality. More recently, coffee has been linked with improved weight management over time.

Most of the health benefits have been shown by drinking three cups of decaf per day.

Moderation is key, and remember that the greatest health benefits will come from having a balanced diet.

The Conversation, 01 November 2023

https://theconversation.com

Scientists Shed New Light on the "Dark Matter" of Cellular Biology

2023-11-17

The findings by professor Samy Cecioni and his students, which open the door to a wide range of applications, were recently published in the prestigious European journal Angewandte Chemie.

Found in all living cells

Sugar is omnipresent in our lives, present in almost all the foods we eat. But the importance of these simple carbohydrates extends far beyond

Researchers at the University of Montreal's Chemistry Department have created an innovative fluorogenic probe for analyzing interactions between sugars and proteins, two families of biomolecules essential to life.

tasty desserts. Sugars are vital to virtually all biological processes in living organisms and there is a vast diversity of naturally occurring sugar molecules.

"All of the cells that make up living organisms are covered in a layer of sugar-based molecules known as glycans," said Cecioni. "Sugars are therefore on the front line of almost all physiological processes and play a fundamental role in maintaining health and preventing disease."

"For a long time," he added, "scientists believed that the complex sugars found on the surface of cells were simply decorative. But we now know that these sugars interact with many other types of molecules, in particular with lectins, a large family of proteins."

Driving disease, from flu to cancer

Like sugars, lectins are found in all living organisms. These proteins have the unique ability to recognize and temporarily attach themselves to sugars. Such interactions occur in many biological processes, such as during the immune response triggered by an infection.

Lectins are attracting a lot of attention these days. This is because scientists have discovered that the phenomenon of lectins "sticking" to sugars plays a key role in the appearance of numerous diseases.

"The more we study the interactions between sugars and lectins, the more we realize how important they are in disease processes," said Cecioni. "Studies have shown how such interactions are involved in bacteria colonizing our lungs, viruses invading our cells, even cancer cells tricking our immune system into thinking they're healthy cells."

Difficult to detect…until now

There are still many missing pieces in the puzzle of how interactions between sugars and lectins unfold because they are so difficult to study. This is because these interactions are transient and weak, making detection a real challenge.

Two of Cecioni's students, master's candidate Cécile Bousch and Ph.D. candidate Brandon Vreulz, had the idea of using light to detect these interactions. The three researchers set to work to create a sort of chemical probe capable of "freezing" the meeting between sugar and lectin and making it visible through fluorescence.

The interaction between sugar and lectin can be described using a "lock and key" relationship, where the "key" is the sugar and the "lock" is the

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lectin. Chemists have already created molecules capable of blocking this lock-and-key interaction and can now to identify exactly what sugars are binding to lectins of high interest to human health.

"Our idea was to label sugar molecules with a chromophore, a chemical that gives a molecule its color," explained Cecioni. "The chromophore is actually fluorogenic, which means that it can become fluorescent if the binding of sugar with the lectin is efficiently captured. Scientists can then study the mechanisms underlying these interactions and the disturbances that can arise."

Cecioni and his students are confident their technique can be used with other types of molecules. It may even be possible to control the color of new fluorescently labeled probes that are created.

By making it possible to visualize interactions between molecules, this discovery is giving researchers a valuable new tool for studying biological interactions, many of which are critical to human health.

Sci Tech Daily, 17 November 2023

https://scitechdaily.com

Chemists use oxygen, copper 'scissors' to make cheaper drug treatments possible

2023-11-22

One chemical used in some anti-cancer drugs, for example, costs pharmaceutical companies $3,200 per gram—50 times more than a gram of gold. The UCLA researchers devised an inexpensive way to produce this drug molecule from a chemical costing just $3 per gram. They were also able to apply the process to produce many other chemicals used in medicine and agriculture for a fraction of the usual cost.

This feat, published in the journal Science, involves a process known as "aminodealkenylation." Using oxygen as a reagent and copper as a catalyst to break the carbon-carbon bonds of many different organic molecules, the researchers replaced these bonds with carbon-nitrogen bonds, converting the molecules into derivatives of ammonia called amines.

Because amines interact strongly with molecules in living plants and animals, they are widely used in pharmaceuticals, as well as in agricultural chemicals. Familiar amines include nicotine, cocaine, morphine and amphetamine, and neurotransmitters like dopamine. Fertilizers, herbicides and pesticides also contain amines.

Drugs to treat cancer are often very expensive to produce, resulting in high costs for the patients who need them. Thanks to pathbreaking research by UCLA chemists, led by organic chemistry professor Ohyun Kwon, the price of drug treatments for cancer and other serious illnesses may soon plummet.

Industrial production of amines is therefore of great interest, but the raw materials and reagents are often expensive, and the processes can require many complicated steps to complete. Using fewer steps and no expensive ingredients, the process developed at UCLA can produce valuable chemicals at a much lower cost than current methods.

"This has never been done before," Kwon said. "Traditional metal catalysis uses expensive metals such as platinum, silver, gold and palladium, and other precious metals such as rhodium, ruthenium and iridium. But we are using oxygen and copper, one of the world's most abundant base metals."

The new method uses a form of oxygen called ozone, a potent oxidant, to break the carbon-carbon bond in hydrocarbons called alkenes, and a copper catalyst to couple the broken bond with nitrogen, turning the molecule into an amine. In one example, the researchers produced a c-Jun N-terminal kinase inhibitor—an anti-cancer drug—in just three chemical steps, instead of the 12 or 13 steps previously needed. The cost per gram can thus be reduced from thousands of dollars to just a few dollars.

In another example, the protocol took just one step to convert adenosine—a neurotransmitter and DNA building block that costs less than 10 cents per gram—into the amine N6-methyladenosine. The amine plays crucial roles in controlling gene expression in cellular, developmental and disease processes, and its production cost has previously been $103 per gram.

Kwon's research group was able to modify hormones, pharmaceutical reagents, peptides and nucleosides into other useful amines, showing the new method's potential to become a standard production technique in drug manufacturing and many other industries.

Phys Org, 22 November 2023

https://phys.org

Discovery of Hemoglobin in the Epidermis Sheds New Light on Our Skin's Protective Properties

2023-11-17

Researchers have shown for the first time that hemoglobin, a protein found in red blood cells, where it binds oxygen, is also present in the epidermis, our skin's outermost body tissue. The study(opens in new tab/window), which appears in the Journal of Investigative Dermatology(opens in new tab/window), published by Elsevier, provides important insights into the properties of our skin's protective external layer.

Research published in the Journal of Investigative Dermatology provides important insights into skin's defense mechanism against aging and cancer

This research was driven by a curiosity about how the epidermis protects our delicate body from the environment and what unexpected molecules are expressed in the epidermis. Researchers discovered the hemoglobin α protein in keratinocytes of the epidermis and in hair follicles. This unexpected evidence adds a new facet to the understanding of the workings of our skin's defense mechanisms.

Lead investigator of the study Masayuki Amagai, MD, PhD, Department of Dermatology, Keio University School of Medicine, Tokyo, and Laboratory for Skin Homeostasis, RIKEN Center for Integrative Medical Sciences, Yokohama, explains: "The epidermis consists of keratinized stratified squamous epithelium, which is primarily composed of keratinocytes. Previous studies have identified the expression of various genes with protective functions in keratinocytes during their differentiation and formation of the outer skin barrier. However, other barrier-related genes escaped prior detection because of difficulties obtaining adequate amounts of isolated terminally differentiated keratinocytes for transcriptome analysis."

Hemoglobin binds gases such as oxygen, carbon dioxide, and nitric oxide, and it is an iron carrier via the heme complex. These properties make epidermal hemoglobin a prime candidate for antioxidant activity and potentially other roles in barrier function.

Professor Amagai continues: "We conducted a comparative transcriptome analysis of the whole and upper epidermis, both of which were enzymatically separated as cell sheets from human and mouse skin. We discovered that the genes responsible for producing hemoglobin were highly active in the upper part of the epidermis. To confirm our findings, we used immunostaining to visualize the presence of hemoglobin α protein in keratinocytes of the upper epidermis."

Professor Amagai concludes: "Our study showed that epidermal hemoglobin was upregulated by oxidative stress and inhibited the production of reactive oxygen species in human keratinocyte cell cultures. Our findings suggest that hemoglobin α protects keratinocytes from oxidative stress derived from external or internal sources such as UV irradiation and impaired mitochondrial function, respectively. Therefore,

the expression of hemoglobin by keratinocytes represents an endogenous defense mechanism against skin aging and skin cancer."

Elsevier, 17 November 2023

https://elsevier.com

Cannabis Chemicals May Have Evolved to Deter Insect Pests

2023-11-16

The study opens the door for potentially developing pesticides from cannabinoid extracts, though such uses would be limited to non-edible plants, given the pharmacological properties of the compounds, which include CBDA, THCA and their precursor CBGA. These compounds are naturally produced by hemp plants and convert to more commonly known CBD, THC and CBG when heated.

In the decades since scientists first identified cannabinoids, research has focused on their medicinal and intoxicating effects, but it's never been clear why these plants evolved cannabinoids in the first place. Researchers have hypothesized that cannabinoids may protect plants from ultraviolet light, pathogens and herbivores.

"It has been speculated that they are defensive compounds, because they primarily accumulate in female flowers to protect seeds, which is a fairly common concept in plants," said Larry Smart, a plant breeder and professor in the School of Integrative Plant Science at Cornell AgriTech in the College of Agriculture and Life Sciences (CALS).

"But no one has put together a comprehensive set of experimental results to show a direct relationship between the accumulation of these cannabinoids and their harmful effects on insects," said Smart, who is the senior author of the study, "Cannabinoids Function in Defense Against Chewing Herbivores in Cannabis Sativa L.," which published on Oct. 13 in the journal Horticulture Research.

"The study gives us insight into how cannabinoids function in natural systems, and can help us develop new THC-compliant hemp cultivars that maintain these natural built-in defenses against herbivores," said George Stack '19, Ph.D. '23, a postdoctoral researcher in Smart's lab and the paper's first author.

The Cornell hemp breeding program started in 2017 by evaluating different commercially available hemp cultivars to see which ones were

Cannabinoids, naturally occurring compounds found in hemp plants, may have evolved to deter pests from chewing on them, according to experiments that showed higher cannabinoid concentrations in hemp leaves led to proportionately less damage from insect larvae.

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best suited for local climate, soils and environment, so recommendations could be made to farmers. Smart, Stack and colleagues noticed that varieties originating from a breeding program in Ukraine were all highly susceptible to Japanese beetles, while other varieties were spared such predation.

"At the end of the season, as we characterized the chemistry of those plants, we learned that the plants from the Ukrainian program did not make any cannabinoids," Smart said.

Since varieties that produced more cannabinoids experienced less predation, the team suspected that the compounds may be acting as a defensive agent to protect hemp plants from insect damage, and they devised experiments to test their hypothesis.

In tests using hemp plants with varying concentrations of cannabinoids, the researchers discovered that damage from leaf-chewing insects (cabbage looper larvae) was higher in leaves with lower levels of cannabinoids.

"In the absence of cannabinoids, we saw heavy insect damage, and in the presence of cannabinoids, we saw much less damage," Smart said.

In controlled feeding studies in the lab, the researchers isolated CBDA and CBGA, and painted the extracts on to an artificial insect diet in a range of concentrations. Larvae grew less and had lower rates of survival as cannabinoid concentration increased, according to the paper.

The Cornell program cannot work with high THCA (the intoxicating compound found in marijuana) plants due to federal restrictions, so THCA as a pesticide was not tested in this research, Smart said.

"The potential use of cannabinoids as a pesticide is an exciting area for future research, but there will certainly be regulatory barriers due to pharmacological activity of the compounds, and more studies are needed to understand what pests cannabinoids will be effective against," Stack said.

Future work will investigate if sap-sucking insects, such as aphids, are also inhibited by cannabinoids. The researchers are also exploring whether species from other plant genera that make cannabinoids, such as the South African woolly umbrella plant (Helichrysum umbraculigerum), could also benefit from their insecticidal properties. If so, it would point

to an example of convergent evolution, where the same adaptation independently arose in different species at different times and locations.

Technology Networks, 16 November 2023

https://technologynetworks.com

All-metal fullerene cluster made for first time

2023-11-22

The football-shaped carbon allotrope buckminsterfullerene (C60), whose unexpected 1985 discovery won Harry Kroto, Robert Curl and Richard Smalley a Nobel prize, has gone on to find use in impact-resistant lightweight materials, solar cells and even medicinal applications. Analogous inorganic fullerene structures have since been produced from compounds such as tungsten disulfide and molybdenum diselenide. But purely metallic fullerenes have remained elusive: theoretical calculations predict that a spherical Au32 form of gold should exist, but – perhaps because of the difficulty of characterising x-ray structures in the gas phase – it has only been detected when stabilised by external ligands.

In the new work, Zhong-Ming Sun at Nankai University in China and colleagues crystallised a compound in which the potassium–gold–antimony [K@Au12Sb20]5- anion is a dodecahedral cluster. A gold atom sits at the centre of each face, with an antimony atom at each vertex. At the centre is a potassium atom, which templates the structure by coordinating to all 12 gold atoms.

Like the original fullerene discovery, the Chinese researchers' findings were unplanned: 'Before we started the experiment we had no idea what would be formed,' says Sun. 'We thought it should be something new but really nobody knew what would happen.'

The molecule's instability may preclude applications, but Sun says the insights it provides into bonding between metal atoms could prove invaluable. 'Nobody thought about forming this kind of structure, but the butterfly shape of the two gold and the two antimony atoms forms a four-centre, two-electron bond,' says Sun; 'This structure can be considered as a kind of super atom because it's spherical aromatic – and this is kind of new.'

'It's a beautiful [study] on the structure of a new metallic molecule with dodecahedral symmetry,' says physical organic chemist Harry Dorn at Virginia Tech; 'I have a feeling it's kind of a stretch to relate it back to a fullerene, because fullerenes can entrap five, six or seven atoms inside.'

A fullerene-like molecule composed entirely of metal atoms has been made by researchers in China. As the molecule is highly unstable, it remains uncertain whether it will find direct applications, but its existence could provide new insights into the bonding between metal atoms.

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Dorn is concerned that the molecule was too unstable for the researchers even to obtain a mass spectrum, but be believes similar molecules might be stabilised in future. He finds the formation mechanism especially interesting: 'I haven't seen anything like that where you go from things that have low symmetry to things that have as high symmetry as this does,' he says. 'I come back to the beauty of it.'

Chemistry World, 22 November 2023

https://chemistryworld.com

Discovery of structural regularity hidden in silica glass

2023-11-21

To uncover more about the structural regularity hidden in glassy materials, a research group has focused on ring shapes in the chemically bonded networks of glass. The group, which included Professor Motoki Shiga from Tohoku University's Unprecedented-scale Data Analytics Center, created new ways in which to quantify the rings' three-dimensional structure and structural symmetries: "roundness" and "roughness."

Using these indicators enabled the group to determine the exact number of representative ring shapes in crystalline and glassy silica (SiO2), finding a mixture of rings unique to glass and ones that resembled the rings in the crystals.

Additionally, the researchers developed a technique to measure the spatial atomic densities around rings by determining the direction of each ring. The study is published in the journal Communications Materials.

They revealed that there is anisotropy around the ring, that is, that the regulation of the atomic configuration is not uniform in all directions, and that the structural ordering related to the ring-originated anisotropy is consistent with experimental evidence, like the diffraction data of SiO2. It was also revealed that there were specific areas where the atomic arrangement followed some degree of order or regularity, even though it appeared to be a discorded and chaotic arrangement of atoms in glassy silica.

"The structural unit and structural order beyond the chemical bond had long been assumed through experimental observations but its identification has eluded scientists until now," says Shiga. "Furthermore, our successful analysis contributes to understanding phase-transitions, such as vitrification and crystallization of materials, and provides the

Glass—whether used to insulate our homes or as the screens in our computers and smartphones—is a fundamental material. Yet, despite its long usage throughout human history, the disordered structure of its atomic configuration still baffles scientists, making understanding and controlling its structural nature challenging.

mathematical descriptions necessary for controlling material structures and material properties."

Looking ahead, Shiga and his colleagues will use these techniques to come up with procedures for exploring glass materials, procedures that are based on data-driven approaches like machine learning and AI.

Phys Org, 21 November 2023

https://Phys.org

Key discovery opens new avenue to lowering cholesterol levels

2023-11-09

High cholesterol is a major risk factor for cardiovascular disease. While statins and dietary changes can lower cholesterol, researchers at UCLA Health have revealed how particular proteins, called Aster proteins, are key to the body's processing of the fat-like substance and may have uncovered a novel approach to cholesterol management.

"Our results show that certain proteins in the Aster family play a critical role in moving cholesterol through the absorption and uptake process," said Peter Tontonoz, corresponding author of the study. "The Aster pathway appears to be a potentially attractive target for limiting intestinal cholesterol absorption and reducing levels of plasma cholesterol."

Intestinal absorption of dietary cholesterol has a major influence on blood cholesterol levels and is a complex, multi-step process. Free cholesterol is drawn into the plasma membrane of enterocytes, the cells that line the inner surface of the intestine, by a protein called Niemann-Pick C1 Like 1 (NPC1L1). It's then moved into another part of the cell called the endoplasmic reticulum, where an enzyme called ACAT2 prepares the cholesterol for packaging and transport in a process called esterification. Cholesterol ester is packaged into chylomicrons for release into the bloodstream and delivery to tissues.

While it was previously understood that NPC1L1 was a key player in the process, what wasn't fully understood was how cholesterol was transported from the exterior of the enterocyte to the endoplasmic reticulum. In the current study, the researchers discovered that when NPC1L1 pulls cholesterol from the intestine into the cell, it triggers the recruitment of Aster proteins resident in the endoplasmic reticulum.

Researchers have identified a previously unknown step in the process by which dietary cholesterol is absorbed from the intestine into the bloodstream. The newfound pathway provides a potential new target for treating high cholesterol.

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"How cholesterol that enters the cell through NPC1L1 reaches the endoplasmic reticulum for esterification and regulation of cholesterol synthesis has been a longstanding mystery," Tontonoz said. "We solve that mystery by showing that two members of the Aster protein family – Aster-B and -C – provide the link between NPC1L1 and ACAT2. By attaching to the plasma membrane, these proteins facilitate cholesterol transport to the endoplasmic reticulum."

Additionally, the researchers found that Aster proteins may provide a new treatment target for controlling cholesterol levels. When they blocked the actions of Aster-B and -C in mice, cellular cholesterol stores dropped, and the processing of cholesterol was impaired.

"These findings highlight the Aster pathway as a physiologically important determinant of dietary lipid absorption that can be targeted pharmacologically," the researchers said.

An existing drug, ezetimibe, targets NPC1L1, inhibits ACAT2 activity and reduces cholesterol absorption. It's sometimes used in combination with statins to reduce blood cholesterol, but it doesn't bind sufficiently to Aster proteins to completely prevent cholesterol transport. The researchers identified an experimental small-molecule drug called AI-3d that directly and potently inhibits Aster-A, -B, and -C, and has been shown, in mice and human cells, to inhibit cholesterol absorption.

The study was published in the journal Science.

New Atlas, 9 November 2023

https://newatlas.com

What Is the New Weight Loss Drug Zepbound, and Why Has It Been Approved?

2023-11-18

The obesity "epidemic"

The World Health Organization has described obesity as an issue of "epidemic proportions". In 2017, 4 million people died as a result of being obese. It's a growing problem in both adults and children, with worldwide obesity tripling since 1975.

Being obese or overweight increases a person's risk of diseases such as heart disease, stroke and diabetes, but research has shown that modest

The US Food and Drug Administration (FDA) has approved Zepbound™ (tirzepatide) for use in conjunction with a reduced-calorie diet and increased exercise to help obese adults manage their bodyweight.

weight loss can prevent progression to type 2 diabetes, improve blood pressure and lower blood cholesterol.

The FDA announced it has granted fast-track approval of Zepbound™ specifically for adults with obesity (defined as a body mass index (BMI) of over 30 kg/m2) or overweight adults with at least one weight-related condition, including high blood pressure, type 2 diabetes or high cholesterol.

It is administered once per week by injection and was shown to be effective for weight loss and management in two randomized, double-blind and placebo-controlled phase 3 trials.

John Sharetts, director of the Division of Diabetes, Lipid Disorders and Obesity at the FDA's Center for Drug Evaluation and Research said, "In light of increasing rates of both obesity and overweight in the United States, today's approval addresses an unmet medical need."

How effective is Zepbound™?

One of the trials looked at the efficacy of Zepbound™ in adults without diabetes, and the other studied adults with diabetes. Participants of both trials were either obese or overweight with a weight-related condition and received the drug or placebo alongside making changes to diet and physical activity.

In both trials, participants receiving either 5, 10 or 15 mg Zepbound saw a statistically significant reduction in bodyweight compared to those receiving the placebo.

In the trial that included people with diabetes, those taking the highest dosage of Zepbound lost 12% of their bodyweight on average. For those without diabetes, this figure was 18% when compared to the placebo group.

Technology Networks, 18 November 2023

https://technologynetworks.com

Study offers new method for determining the water content of water-soluble compounds

2023-11-21

In pharmaceutical research and development, it is very important to know the exact structure and water content of the compound being studied, as they affect both the physicochemical and pharmaceutical properties of the compound. Additionally, the water content affects the total molecular weight of the compound that is needed for the calculation of the correct drug dosage.

Researchers at the University of Eastern Finland School of Pharmacy have developed a new method for the accurate determination of the water content of water-soluble compounds. This plays a significant role in, for example, drug dosage. The method utilizes solution-state nuclear magnetic resonance spectroscopy, that is, NMR spectroscopy. The study was published in Analytical Chemistry.

There are several methods for determining the water content of chemical compounds, of which titration and thermogravimetry (TGA) are the most common ones. However, most methods require accurate weighing, destroy the sample, require special expertise or are time-consuming.

The NMR method developed in the study is simple and accurate and works very well for determining the water content of water-soluble compounds, as the NMR results were comparable with the water contents obtained by TGA and X-ray crystallography determinations.

"The research also revealed that the previously determined water content may change during storage. For example, the commercial sodium salt of citric acid had changed from a form containing 5.5 crystal water molecules to one containing 2 crystal water molecules," Senior Researcher Tuulia Tykkynen and Senior Researcher Petri Turhanen of the University of Eastern Finland point out.

The advantages of the NMR method are easy sample handling (no accurate weighing required), speed (the measurement of one sample and the calculation of the result takes about 15–20 minutes) and the possibility of recovering the investigated compound after the measurement, as the method does not destroy the sample.

The method is also sufficiently precise and repeatable. An NMR spectrometer is a very expensive investment, but it can be stated that the equipment in question is almost always found in laboratories where new compounds and pharmaceuticals are synthesized, as it is an essential tool for structure determinations.

Phys Org, 21 November 2023

https://phys.org

New tech screens & identifies drugs capable of stopping melanoma spread

2023-11-21

Metastatic cancers, particularly melanoma, continue to present a challenge because each tumor may have a unique microenvironment and respond differently to treatment. A particularly aggressive form of cancer, once melanoma has spread, its survival rate is low.

A feature of the metastatic process is the formation of invadopodia by tumor cells, specialized protrusions whose function is to degrade the extracellular matrix so that the cells can enter – or invade – new environments. Identifying drugs that target invadopodia is crucial to effectively preventing cancer spread, but currently, the ability to screen for these drugs is lacking.

All that might've changed with the development of "Invasion-Block," an automated, high-content screening platform that's enabled researchers at the Centenary Institute in Australia to assess how well various drugs and compounds can prevent the spread of melanoma by targeting invadopodia.

"Melanoma is a tough opponent, often spreading rapidly and making it difficult to treat," said Shweta Tikoo, the study's corresponding author. "The key to finding better treatments lies in drug discovery, and this is where the 'Invasion-Block' tool plays a pivotal role."

The researchers combined Invasion-Block with an automated image analysis pipeline adapted from astronomical sciences called Smoothen-Mask and Reveal (S-MARVEL), which was used to remove artifacts and substantially improve the quality of datasets of microscopic images of invadopodia.

They then screened 3,840 drugs in two FDA-approved compound libraries for their ability to inhibit invadopodia formation in melanoma cells and found that the most effective compounds were kinase inhibitors. A kinase inhibitor blocks the action of protein kinases, which add a phosphate group to a protein in a process called phosphorylation. Phosphorylation can turn a protein on or off, affecting its level of activity and function, and is often a required step in the growth of some cancers.

"This suggests these enzymes may hold the key to finding treatments that can help curb the spread of melanoma," said Dajiang Guo, lead author of the study.

Researchers have developed an automated platform that they've used to screen thousands of drugs and identify those that can be used to interrupt the spread of melanoma, one of which they successfully trialed on mice. The approach could help identify promising drugs to treat metastatic cancers.

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Of the identified kinase inhibitors, the researchers chose to test the effectiveness of the ataxia-telangiectasia mutated (ATM) inhibitor in the lab. They used CRISPR gene-editing technology to knock out the gene responsible for expressing ATM kinase in melanoma cells and found that the cells became less invasive and didn't spread to the lymph nodes in mice as much.

"We believe that ATM may serve as a potent therapeutic target for treating the spread of melanoma in patients," said Tikoo.

The study is a significant step forward in the fight against melanoma, the researchers say, laying the groundwork for future studies and the development of novel treatments.

"The combination of 'Invasion-Block' and 'S-MARVEL' is opening new avenues in the search for drugs that can arrest the spread of cancer," Tikoo said.

New Atlas, 21 November 2023

https://newatlas.com

New Insights Into DNA Repair Pathway Implicated in Breast, Ovarian and Prostate Cancers Revealed

2023-11-16

Our DNA is not indestructible. Throughout the course of our lives, DNA can break in response to natural and environmental factors. Thankfully, our bodies have dedicated enzymes and pathways which can glue our broken DNA back together through several different mechanisms, known as DNA repair pathways.

Some cancers, however, can hijack these pathways for their own benefit. Susanna Stroik, PhD, and Dale Ramsden, PhD, both researchers in the Department of Biochemistry and Biophysics in the UNC School of Medicine and the UNC Lineberger Comprehensive Cancer Center, have pieced together the lesser-known DNA repair pathway, called polymerase theta-mediated end joining (TMEJ).

The pathway - which has been found to be upregulated in many patients with hereditary breast cancer, ovarian cancer, and prostate cancer, specifically those involving BRCA1 and BRCA2 mutations - has been laid out step by step in a published article in Nature, and the new knowledge could lead to new therapies for cancer.

A lesser-known DNA repair pathway that is upregulated in breast, ovarian and prostate cancer has been pieced together.

"People with these breast cancer mutations, their cancers rely on polymerase theta's repair pathway to keep the tumors alive and repair DNA damage in the cancerous tissue," said Stroik, a postdoctoral researcher in Ramsden's lab. "Now that we know more about this pathway, scientists could, in theory, produce a drug that could disrupt key pieces of the pathway in cancer cells, as opposed to using conventional chemotherapies that destroy healthy cells along with the cancer."

Polymerase Theta's Discovery

Out of all DNA repair pathways, TMEJ has been the most elusive. Richard Wood, PhD, a distinguished professor at University of Texas MD Anderson Cancer Center played a key role in the first characterization of polymerase theta in 2003.

Over the next 15 years, multiple labs, including the Wood, Ramsden, and Gupta labs (also at Lineberger Comprehensive Cancer Center), were able to link polymerase theta to DNA repair (TMEJ) and cancer. Sylvie Doublié, PhD, an alumnus of UNC-Chapel Hill and professor of microbiology and molecular genetics at the University of Vermont, then solved the first structure of polymerase theta.

Technology Networks, 16 November 2023

https://technologynetworks.com

New carbon material sets energy-storage record, likely to advance supercapacitors

2023-11-22

"By combining a data-driven method and our research experience, we created a carbon material with enhanced physicochemical and electrochemical properties that pushed the boundary of energy storage for carbon supercapacitors to the next level," said chemist Tao Wang of ORNL and the University of Tennessee, Knoxville.

Wang led the study, titled "Machine-learning-assisted material discovery of oxygen-rich highly porous carbon active materials for aqueous supercapacitor" and published in Nature Communications, with chemist Sheng Dai of ORNL and UTK.

"This is the highest recorded storage capacitance for porous carbon," said Dai, who conceived and designed the experiments with Wang. "This is a real milestone."

Guided by machine learning, chemists at the Department of Energy's Oak Ridge National Laboratory designed a record-setting carbonaceous supercapacitor material that stores four times more energy than the best commercial material. A supercapacitor made with the new material could store more energy—improving regenerative brakes, power electronics and auxiliary power supplies.

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The researchers conducted the study at the Fluid Interface Reactions, Structures and Transport Center, or FIRST, an ORNL-led DOE Energy Frontier Research Center that operated from 2009 to 2022. Its partners at three national labs and seven universities explored fluid-solid interface reactions having consequences for capacitive electrical energy storage. Capacitance is the ability to collect and store electrical charge.

When it comes to energy storage devices, batteries are the most familiar. They convert chemical energy to electrical energy and excel at storing energy. By contrast, capacitors store energy as an electric field, akin to static electricity. They cannot store as much energy as batteries in a given volume, but they can recharge repeatedly and do not lose the ability to hold a charge. Supercapacitors, such as those powering some electric buses, can store more charge than capacitors and charge and discharge more quickly than batteries.

Commercial supercapacitors have two electrodes—an anode and cathode—that are separated and immersed in an electrolyte. Double electrical layers reversibly separate charges at the interface between the electrolyte and the carbon. The materials of choice for making electrodes for supercapacitors are porous carbons. The pores provide a large surface area for storing the electrostatic charge.

The ORNL-led study used machine learning, a type of artificial intelligence that learns from data to optimize outcomes, to guide the discovery of the superlative material. Runtong Pan, Musen Zhou and Jianzhong Wu from the University of California, Riverside, a FIRST partner university, built an artificial neural network model and trained it to set a clear goal: develop a "dream material" for energy delivery.

The model predicted that the highest capacitance for a carbon electrode would be 570 farads per gram if the carbon were co-doped with oxygen and nitrogen.

Wang and Dai designed an extremely porous doped carbon that would provide huge surface areas for interfacial electrochemical reactions. Then Wang synthesized the novel material, an oxygen-rich carbon framework for storing and transporting charge.

The carbon was activated to generate more pores and add functional chemical groups at sites for oxidation or reduction reactions. Industry uses activation agents such as potassium hydroxide that require a very high temperature, around 800°C, which drives oxygen from the material. Five years ago, Dai developed a process using sodium amide as the activation

agent. It works at a lower temperature, near 600°C, and creates more active sites than the hotter industrial process. "Material synthesis in this 'Goldilocks zone'—not too cold, not too hot—made a real difference in not decomposing the functional groups," Dai said.

The synthesized material had a capacitance of 611 farads per gram—four times higher than a typical commercial material. Pseudocapacitance is storage of charge based on continuous, fast and reversible oxidation-reduction reactions at the surface of electrode materials. Pseudocapacitance from such reactions at the oxygen/nitrogen sites contributed to 25% of the overall capacitance. The material's surface area was among the highest recorded for carbonaceous materials—more than 4,000 square meters per gram.

This success came quickly. The data-driven approach allowed Wang and Dai to achieve in three months what would have previously taken at least a year.

"We achieved the performance of carbon materials at the limit," Wang said. "Without the goal that machine learning set, we would have kept optimizing materials through trial and error without knowing their limit."

The key to success was achieving two kinds of pores—mesopores between 2 and 50 nanometers, or billionths of a meter, and micropores tinier than 2 nanometers. In experimental analyses, the chemists found that the combination of mesopore and micropores provided not only a high surface area for energy storage but also channels for electrolyte transport. Miaofang Chi and Zhennan Huang at the Center for Nanophase Materials Sciences, a DOE Office of Science user facility at ORNL, performed scanning transmission electron microscopy to characterize the mesopores, but the micropores were too small to see.

Microscopically, the material looks like a golf ball with deep dimples. The dimples represent mesopores, and the micropores exist in the material between the dimples.

"You are building a highway for ion transport," Dai said. "Supercapacitors are all about high-rate performance—fast charging, fast discharging. In this structure that Tao and I designed, you have a larger pore, which you can view as a superhighway. This is connected to smaller roads, or tinier pores."

"The smaller pores provide a larger surface for storing charge, but the larger pores are like a highway that can speed up the charge/discharge

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rate performance," Wang said. "A balanced amount of small and large pores can realize the best performance, as predicted by the artificial neural network model."

To characterize the electrolyte's transport in the carbon pores, Murillo Martins and Eugene Mamontov of the Spallation Neutron Source, a DOE Office of Science user facility at ORNL, performed quasielastic neutron scattering. "They tracked the speed on the highway," Wang said. "This was the first time that neutron scattering was used to analyze diffusion of a sulfuric acid electrolyte in the confined spaces of carbon nanopores." Neutron scattering revealed the electrolyte moved at different speeds: quickly in the mesopores and slowly in the micropores.

Wang quantified the capacitance contributions from pores of different sizes and oxidation-reduction reactions at their surfaces via modified step potential electrochemical spectroscopy, a technique that can be done in only a few places in the world. "We found that mesopores doped with oxygen and nitrogen contribute most to the overall capacitance," Wang said.

The FIRST team performed other studies of the physicochemical properties. Jinlei Cui and Takeshi Kobayashi from Ames National Laboratory used nuclear magnetic resonance to analyze the structure of polymer precursors. Bishnu Thapaliya of ORNL and UTK conducted Raman analysis, revealing the carbon's amorphous, or disordered, structure.

Zhenzhen Yang of UTK and ORNL and Juntian Fan of UTK participated in the surface area measurements.

This research has the potential to accelerate the development and optimization of carbon materials for supercapacitor applications. Although this breakthrough study used the best data at the time, scientists now have even more boundary data for training the machine learning model for the next study.

"Using more data, we can set a new target and push the boundaries of carbon supercapacitors even further," Wang said. "The successful application of machine learning in materials design is a testament to the power of data-driven approaches in advancing technology."

Phys Org, 22 November 2023

https://phys.org

Slow-release diabetes drugs could cut shots from daily to 3 times a year

2023-11-21

An effective and relatively recent form of diabetes treatment involves drugs that mimic a hormone called glucagon-like peptide 1 (GLP-1), which manages insulin release and reduces appetite. These include FDA-approved drugs like Ozempic and Mounjaro, which also seem to have the bonus benefit of weight loss. These drugs are usually administered weekly, while the more familiar insulin shots are needed daily. Either way, that strict routine can be quite a burden on patients – and this is the problem that the Stanford team is tackling.

"Adherence is one of the biggest challenges in Type 2 diabetes management," said Eric Appel, principal investigator on the study. "Needing only three shots a year would make it much easier for people with diabetes or obesity to stick with their drug regimens."

To achieve this, the team developed a hydrogel that can be infused with GLP-1 molecules, then injected under the skin. Once there, it slowly dissolves and releases the drugs at the right dose for an extended period of time. The scientists designed the hydrogel so that it could be fluid enough to be injected using regular syringes, but stable enough to last several months – and for the drug depot to be small enough to not cause discomfort in the patient.

In tests in rats with type 2 diabetes, injections of the drug-loaded hydrogel once every 42 days resulted in better management of blood glucose and weight than daily shots of conventional drugs.

That 42-day routine in rats is the equivalent of four months in humans, the team says. This timeframe was chosen to coincide with the usual checkup regimen, meaning patients could get their shots as part of routine doctor visits. However, the researchers say they've been able to tune the hydrogel to release drugs over a few days or even up to six months, which could make it a solid delivery system for a range of other drugs like anti-inflammatories or cancer therapies.

The next round of tests will be conducted in pigs, because they have more human-like skin and endocrine systems. Human trials could begin in as little as 18 months to two years, the team says.

New Atlas, 21 November 2023

https://newatlas.com

Managing diabetes usually involves regular shots of insulin or other drugs, but soon patients might only need to inject themselves a few times a year.

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Coffee grounds transform into quantum dots to treat dementias

2023-11-23

Carbon quantum dots, made from caffeic acid in used coffee, have shown promise in lab-based tests to protect brain cells from substances that can cause these diseases.

While still in its early stages, the research could herald an environmentally friendly way to neurodegenerative diseases that have been caused by environmental factors, like age or exposure to toxins (like the pesticide paraquat).

"Caffeic-acid based carbon quantum dots have the potential to be transformative in the treatment of neurodegenerative disorders," says Jyotish Kumar, a doctoral student at the University of Texas at El Paso and lead author on a paper published in Environmental Research.

"This is because none of the current treatments resolve the diseases; they only help manage the symptoms. Our aim is to find a cure by addressing the atomic and molecular underpinnings that drive these conditions."

Quantum dots, a concept which won this year's Nobel Prize in Chemistry, are crystals the size of nanometres (on the same scale as molecules). The team made these quantum dots with purchased caffeic acid, but they point out it's been made before by extraction from used coffee grounds.

In their early stages, many neurodegenerative diseases share chemical features, particularly if they've been caused by environmental factors. People have higher levels of molecules called free radicals in their system, and they also have a build up of a type of protein (amyloid proteins) in the brain.

Caffeic acid is an antioxidant, which neutralises free radicals. It's also capable of getting from our blood stream into our brains (crossing the "blood-brain barrier"), so the researchers thought it could be an effective medication.

"It is critical to address these disorders before they reach the clinical stage," says co-author Professor Mahesh Narayan, also at the University of Texas at El Paso.

"At that point, it is likely too late. Any current treatments that can address advanced symptoms of neurodegenerative disease are simply beyond the means of most people.

Scientists have turned old coffee grounds into a substance that could prevent Alzheimer's, Parkinson's and other neurodegenerative diseases.

"Our aim is to come up with a solution that can prevent most cases of these conditions at a cost that is manageable for as many patients as possible."

The researchers tested their quantum dots on cell lines that had had Parkinson's disease induced by paraquat. The caffeic acid both removed free radicals and prevented amyloid proteins building up.

The researchers are now seeking funding to see if they can take the substance to pre-clinical trials – the first step on the long road towards a medication.

Cosmos, 23 November 2023

https://cosmosmagazine.com

Drug Approved To Prevent Breast Cancer Post-Menopause in the UK

2023-11-07

The Medicines and Healthcare products Regulatory Agency (MHRA) has today authorised this new indication for Anastrozole, a hormone treatment used for breast cancer in post-menopausal women.

Anastrozole was already authorised for use in the treatment of breast cancer in post-menopausal women and has been used off-label for prevention.

Today's announcement confirms the authorisation for prevention in post-menopausal women at moderate or high risk of developing the disease.

Evidence was based on the IBIS-II study, an international, randomised double-blind, placebo-controlled trial, which showed fewer women developed breast cancer in the anastrozole group compared to the placebo group.

Breast cancer is the most common type of cancer in the UK. Most women diagnosed with breast cancer are over the age of 50, but younger women can also get breast cancer. Around 1 in 7 women will be diagnosed with breast cancer in their lifetime.

The treatment is taken as a 1mg tablet, once a day for 5 years.

Anastrozole is an aromatase inhibitor. This works by cutting down the amount of the hormone oestrogen that a patient's body makes by blocking an enzyme called 'aromatase'.

Anastrozole is now authorised as a pre-ventative treatment for post-menopausal women at high risk of breast cancer.

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The most common side effects of the medicine are hot flushes, feeling weak, pain/stiffness in the joints, arthritis, skin rash, nausea, headache, osteoporosis, and depression.

As with any medicine, the MHRA will keep the safety and effectiveness of Anastrozole under close review. Anyone who suspects they are having a side effect from this medicine are encouraged to talk to their doctor, pharmacist or nurse and report it directly to the Yellow Card scheme, either through the website or by searching the Google Play or Apple App stores for MHRA Yellow Card.

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Technology Network, 07 November 2023

https://technologynetwork.com

Researchers create molecule to tackle antimicrobial resistance

2023-11-21

Antimicrobial Resistance (AMR) occurs when bacteria, viruses, fungi, and parasites change over time and no longer respond to medicines, making infections harder to treat and increasing the risk of disease, severe illness, and death. The development of new ways to kill bacteria is an urgent scientific need, as most conventional antibiotics will no longer be effective in 2050 due to the rising levels of AMR.

The research harnessed the principles of supramolecular chemistry, a niche scientific area that explores interactions between molecules, to achieve the breakthrough. Most importantly, the study uncovered molecules that are efficient at killing bacteria but whose toxicity to healthy human cells is very low.

The new research is described in Chem, to coincide with World AMR Awareness Week which runs from 18–24 November. This global campaign, run by the World Health Organization, aims to raise awareness and understanding of AMR in the hope of reducing the emergence and spread of drug-resistant infections.

More than 1.2 million people, and potentially millions more, died in 2019 as a direct result of antibiotic-resistant bacterial infections, according to the most comprehensive estimate to date of the global impact of AMR.

Researchers at Maynooth University, working as part of an international team, have created a new molecule that could help in the fight against drug-resistant bacteria.

This research may pave the way for new approaches to tackle this problem that kills more people annually than HIV/AIDS or malaria.

Lead researcher Luke Brennan of Maynooth University's Department of Chemistry said, "We are discovering new molecules and looking at how they bind to anions, which are negatively charged chemicals that are extremely important in the context of the biochemistry of life. We are laying the fundamental foundations that could prove useful in combating various diseases from cancer to cystic fibrosis."

The work is based on the use of synthetic ion transporters and is the first time that researchers have demonstrated that an influx of salt (sodium and chloride ions) into the bacteria can cause a series of biochemical events that lead to bacterial cell death—even in strains that are resistant to currently available antibiotics such as methicillin-resistant Staphylococcus aureus (MRSA).

Study co-author Dr. Robert Elmes of Maynooth University's Kathleen Lonsdale Institute for Human Health Research says, "This work shows how using our approach, a sort of 'trojan horse' that causes an influx of salt into cells, we can effectively kill resistant bacteria in a way that counteracts known methods of bacterial resistance."

Bacteria work hard to maintain a stable concentration of ions inside their cell membranes, and when this delicate balance is disrupted, it wreaks havoc on normal cell function, and the cells cannot survive.

Elmes says, "These synthetic molecules bind to chloride ions and wrap it up in a 'fatty blanket' that allows it to easily dissolve in the bacteria's membranes, bringing the ions along for the ride and disrupting the normal ionic balance. The work is a great example of foundation knowledge in chemistry fundamentals impacting on unmet needs in human health research."

Prof Kevin Kavanagh, a microbiologist in Maynooth University's Department of Biology, says, "The rising incidence of infections by drug-resistant bacteria is a major concern. This work is an example of cheists and biologists working together to pioneer the development of new antimicrobial agents with significant future potential."

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Such results pave the way for the potential development of anion transporters as a viable alternative to currently available antibiotics, something urgently required as the problem of AMR continues to rise.

Phys Org, 21 November 2023

https://Phys.org

Simple New Technique Transforms "Forever Chemicals" Into Valuable Compounds

2023-11-16

Commonly known as "forever chemicals," PFAS (Perfluoroalkyl and Polyfluoroalkyl Substances) are notorious for their persistence in both the environment and our bodies. However, chemists from Osaka Metropolitan University have developed a simple yet innovative technique that can transform these harmful substances into valuable compounds.

Breakthrough in PFAS Conversion

A research group led by Professor Masato Ohashi and Assistant Professor Kenichi Michigami of the Graduate School of Science at Osaka Metropolitan University has successfully synthesized ligands called fluorine-decorated N-heterocyclic carbenes (NHCs) from perfluoroalkenes, a type of PFAS (Perfluoroalkyl and Polyfluoroalkyl Substances).

Scientists have developed an innovative approach to incorporate harmful perfluoroalkenes into N-heterocyclic carbene ligands.

The NHCs developed in this study play significant roles in stabilizing unstable molecules as well as enhancing the performance of their ligated transition metal complexes.

The Process of Synthesis

The synthesis of fluorinated NHCs was achieved simply by removing two fluorine atoms from 1,2-difluoroalkene derivatives. Owing to the small size of fluorine atoms, the electron-accepting ability of the NHC ligand can be enhanced without substantially changing its steric properties.

"Our results enable the easy transformation of harmful PFAS into functional NHCs," explained Dr. Michigami. "The versatile applications of fluorinated NHCs show potential advantages in various fields such as fluorine chemistry, organometallic chemistry, catalysis chemistry, and materials science."

SciTechDaily, 16 November 2023

https://scitechdaily.com

Thank gluten's complex chemistry for your light, fluffy baked goods

2023-11-21

I'm a chemist who teaches a chemistry of cooking class, and every year I ask my students, "What is gluten?" Common answers are "a sugar" or "a carbohydrate." But rarely does anyone get it right.

So, what is gluten?

Gluten is a complex mixture of proteins. It makes up 85%-90% of the protein in flour. Proteins are natural biological macromolecules composed of chains of amino acids that fold upon themselves to adopt a variety of shapes.

Gluten comes from the endosperm of wheat, rye, barley and related plants. The endosperm is a tissue in the plant's seeds that serves as a storage location for starch and protein. The milling process that creates flour releases the contents of the endosperm, including gluten.

The main proteins in the gluten mixture are gliadin and glutenin. These proteins make up much of flour-based food products' structure. During the kneading or mixing part of making dough, these proteins form an elastic mesh, often referred to as the gluten network.

Creating a gluten network

Forming a gluten network is key for getting dough to rise. The network acts as a balloon that traps gases during the rising, proofing and baking processes. During rising and proofing, when the dough is given time to expand, yeast in the dough releases carbon dioxide as it eats and digests the sugars present. This process is called fermentation.

The baking process produces a number of different gases, such as carbon dioxide, water in the form of steam, ethanol vapors and nitrogen. The gluten network traps these gases and the dough expands like a balloon. If the gluten network is too strong, the gases will not produce enough pressure to make the dough rise. If it's too weak, the balloon will burst and the dough will not stay risen. How strong the gluten network ends up being depends on how long you knead and mix the dough.

For the gluten network to form, you need to knead or mix the dough with some water – this aligns the proteins.

Within the bread, rolls and baked goods on many tables this holiday season is an extraordinary substance – gluten. Gluten's unique chemistry makes foods airy and stretchy.

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The glutenin proteins come in long and short chains that adopt coiled structures. These coils are held together through attractive forces between the loops of the coils known as intramolecular hydrogen bonds. Kneading and mixing break some of the attractive forces and align the glutenin proteins.

Bonds form between the individual glutenin chains through sulfur atoms on some of the amino acids that make up glutenin. When these amino acids – called cysteines – are brought into contact with each other, the sulfur atoms bond to one another, creating a linkage called a disulfide bond.

As more and more cysteines form disulfide bonds with cysteines on neighboring proteins, the network grows. So, the more proteins present and the longer the kneading process, the stronger the gluten network. Bread flour has higher protein concentrations – 12%-14% – than other flours, so bread flour leads to a stronger gluten network and more rise.

The gliadin proteins are smaller and more compact than glutenin proteins. During the kneading process, gliadin disperses throughout the glutenin polymers. While glutenin provides elasticity and strength to dough, the gliadin proteins make the dough viscous, or fluidlike, and dense.

Strengthening and shortening

Adding salt neutralizes any charges that may be present on the proteins. This minimizes any repulsion between the proteins and brings them closer together. This process forces water out from between the proteins, which both brings the proteins closer together and stabilizes the network. So, adding salt will create a stronger network that increases the amount of stretching and pulling the dough can withstand.

Fats like butter or margarine will weaken, or "shorten," the gluten network. Typically, recipes ask you to mix the fats with the flour before adding water or milk. This is so the fats coat the flour. And because fats are hydrophobic, or water-repellent, this process prevents the water that helps the gluten network form from reaching the proteins. This results in a softer, more tender baked good.

Without the formation of the gluten network, baked goods would not rise into the light and fluffy delicious dishes we love.

The Conversation, 21 November 2023

https://theconversation.com

UK becomes first country in the world to authorise a Crispr-based gene therapy

2023-11-17

The UK's drug agency has become the first in the world to authorise a Crispr gene-editing therapy. The new treatment has been approved for sickle-cell disease and transfusion-dependent β-thalassaemia and has the potential to cure patients with these conditions.

Both genetic conditions are caused by errors in the genes for haemoglobin, a protein found in red blood cells which carries oxygen around the body. Casgevy, manufactured by Vertex Pharmaceuticals and Crispr Therapeutics, uses Crispr to alter a specific gene in a patient's bone marrow stem cells called BCL11A, to enable the production of a functioning haemoglobin.

To do this, stem cells are taken from the patient's bone marrow and edited in a laboratory. Patients must then undergo conditioning treatment to prepare the bone marrow before the modified cells are infused back into the patient. The results of the treatment have the potential to be lifelong.

Casgevy has been authorised by the Medicines and Healthcare products Regulatory Agency (MHRA) for patients from 12 years old for whom haematopoietic stem cell transplantation is an appropriate treatment but a suitable donor is not available. Vertex and Crispr Therapeutics estimate that 2000 patients will be eligible for treatment in the UK.

'Both sickle cell disease and β-thalassaemia are painful, life-long conditions that in some cases can be fatal,' said Julian Beach, interim executive director of healthcare quality and access at the MHRA. 'To date, a bone marrow transplant – which must come from a closely matched donor and carries a risk of rejection – has been the only permanent treatment option.'

Fast-tracked treatment

The decision to authorise the Crispr treatment was based on a review of the available evidence including interim outcomes from two ongoing trials. In the sickle cell disease trial, 45 patients have received Casgevy, although only 29 patients have been on the trial long enough to qualify for the primary efficacy interim analysis. Of these patients, 97% were free of painful blood vessel blockages that characterise these diseases for at least 12 months after treatment.

Treatment aims to cure patients with β-thalassaemia and sickle-cell disease

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In the transfusion-dependent β-thalassaemia trial, 54 patients received Casgevy, with 42 included in the interim analysis. Of these, 93% did not need a red blood cell transfusion for at least a year after treatment and the remaining three had more than a 70% reduction in the need for transfusions.

Alena Pance, a senior lecturer in genetics at the University of Hertfordshire, said the authorisation was a 'great step' to tackle genetic diseases 'we never thought would be possible to cure'.

'Modifying the stem cells from the bone marrow of the patient avoids the problems associated with immune compatibility, ie searching for donors that match the patient and following immunosuppression, and constituting a real cure of the disease rather than a treatment,' she added.

'The exciting aspect of this is the strategy used for the gene editing because blood diseases can be caused by a number of different mutations that it would be difficult to target individually. This therapy relies on switching off a transcription factor (BCL11A), which is a protein that enables the transition from foetal haemoglobin to adult haemoglobin at birth. This results in the making of foetal haemoglobin that can overcome the defects or absence of the adult beta globin, which makes this approach applicable independently of the specific mutation affecting beta globin present in individual patients.'

Steve Bates, chief executive of the UK Bioindustry Association, said the UK was 'well set' to be the first place in the world to license, manufacture and provide access to gene editing treatments via an 'equitable health system'. 'Not only do we have today's world first regulatory approval via the MHRA but we already have in place the NHS innovative medicine fund as an explicit policy route to enable rapid adoption of innovation,' he added.

In the UK, Casgevy was granted an MHRA 'innovation passport' which helps to speed up the approval process with the aim of getting treatments to patients sooner. Vertex said it was already working closely with national health authorities to secure access for eligible patients 'as quickly as possible', although it has not yet disclosed the treatment's price.

Chemistry World, 17 November 2023

https://chemistryworld.com

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Technical Notes

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Exposure concentration ratios and biological responses play a critical role in determining the joint toxicity of TiO2 nanoparticles and As(V) to the organism: The case study in marine algae Phaeodactylum tricornutum

Spatial heterogeneity and compositional profiles of dissolved organic matter in farmland soils across mainland China

ENVIRONMENTAL RESEARCH

Nano-size cobalt-doped cerium oxide particles embedded into graphitic carbon nitride for enhanced electrochemical sensing of insecticide fenitrothion in environmental samples: An experimental study with the theoretical elucidation of redox events

Reporting and reproducibility: Proteomics of fish models in environmental toxicology and ecotoxicology

PHARMACEUTICAL/TOXICOLOGY

Adverse impacts of environmentally relevant PFOS alternatives on mice pancreatic tissues

Long-term exposure to polystyrene microplastics induces hepatotoxicity by altering lipid signatures in C57BL/6J mice

Binary metal oxide (NiO/SnO2) composite with electrochemical bifunction: Detection of neuro transmitting drug and catalysis for hydrogen evolution reaction

OCCUPATIONAL

The impact of short-term exposures to ambient NO2, O3, and their combined oxidative potential on daily mortality

Population pharmacokinetic/pharmacodynamic modeling and exposure-response analysis of ciprofol in the induction and maintenance of general anesthesia in patients undergoing elective surgery: A prospective dose optimization study