CHEMWATCH

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ASIA PACIFIC

Japan's PAC List Updated: Six Substances Added and Six Removed

2023-05-22

According to the Gazette on April 3, 2023, Japan added six substances to the List of Priority Assessment Chemical Substances (PACs) following the removal of six substances on March 31. This brings the total number of PACs to 218.

The details of changes to the list are presented in the table below:

	Substance name
Six substances added into list	Sodium salt of 2,2′ ,2″,2‴-(ethane-1,2-diyldinitrilo)tetraacetic acid
	alpha,alpha′-[(Alkyl(C=8-18, normal chain)azanediyl)bis(ethane-2,1-diyl(or methylethane-2,1-diyl))]bis{omega-hydroxypoly[oxyethane-1,2-diyl/oxy(methylethane-1,2-diyl)]} (The repeating number of repeating unit is an integer 1 or more.) (It is limited that the number-average molecular weight of the polymer is less than 1,000.)
	Salt of {ester of 2-hydroxy-N-(2-hydroxyethyl)-N,N-dimethylethan-1-aminium and [saturated fatty acid(C=10-18, normal chain) (or unsaturated fatty acid(C=18, normal chain))]} or salt of {ester of 2-hydroxy-N-(2-hydroxypropyl)-N,N-dimethylpropan-1-aminium and [saturated fatty acid(C=10-18, normal chain)(or unsaturated fatty acid(C=18, normal chain))]}
	alpha-(Alkyl(C=6-18))-omega-hydroxypoly[oxyethane-1,2-diyl/oxy(methylethane-1,2-diyl)](It is limited that the number-average molecular weight of the polymer is less than 1,000.)
	alpha-Hydro-omega-[(3-methylbut-3-en-1-yl)oxy]poly(oxyethane-1,2-diyl) (The repeating number of repeating unit is an integer 1 or more.) (It is limited that the number-average molecular weight of the polymer is less than 1,000.)
	[alpha-(Alkanoyl(C=8-18, normal chain))-omega-methoxypoly(oxyethane-1,2-diyl) or alpha-(alkenoyl(C=8-18, normal chain))-omega-methoxypoly(oxyethane-1,2-diyl)] (The repeating number of repeating unit is an integer 1 or more.) (It is limited that the number-average molecular weight of the polymer is less than 1,000.)
Six substances removed from the list (now classified as general chemicals)	Methyl dodecanoate
	o-Dichlorobenzene
	Ethylamine
	Benzyl benzoate
	Camphene
	Chlorodifluoromethane

Under the framework of Chemical Substance Control Law (CSCL), manufacturers and importers of PACs need to report to the Ministry of Economy, Trade and Industry (METI) during the period from April to June each year the production and/or import volume in the previous calendar year, the use category, and the production site, etc.

It should be noted that the six deleted substances and the six added substances can be reported as general chemicals this year.

The PACs list is accessible here.

Read More

REACH24, 22-05-23

https://www.reach24h.com/en/news/industry-news/chemical/japans-pac-list-updated-6-substances-added-and-6-removed.html

Consultation on proposed changes to infant formula standards

2023-05-24

We're calling for public submissions on our assessment of Code standards for infant formula products.

The review aims to ensure regulation of infant formula is clear, reflects the latest scientific evidence and aligns with international standards.

This is the second round of consultations under Proposal P1028 - Infant formula.

This review covers infant formula (for use from newborn), follow-on formula (for use from six to 12 months of age) and infant formula for special dietary use.

Although breastfeeding is the recommended way to feed a baby, a safe and nutritious substitute for breast milk is needed for babies who are not breastfed.

To find out more or have your say, see our website.

Read More

ANZ Food Standards Code, 24-05-23

https://mailchi.mp/ef6438295cef/food-standard-news-1300748

Public consultations

2023-05-23

Application A1262 – Food derived from insect-protected corn line MON95275

FSANZ invites written submissions on the assessment of food derived from corn line MON95275, genetically modified for protection from coleopteran insect pests. Submissions close 6pm (Canberra time) 18 May 2023.

Application A1264 – Food derived from drought-tolerant and herbicide-tolerant soybean line IND-00410-5

FSANZ invites written submissions on the assessment of food derived from soybean line IND-00410-05, genetically modified for drought and herbicide tolerance. Submissions close 6pm (Canberra time) 7 June 2023.

Proposal P1028– Infant Formula

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FSANZ invites written submissions on the assessment of the revision and clarification of standards relating to infant formula products comprising category definitions, composition, labelling and representation of products. Submissions close 6pm (Canberra time) 7 July 2023.

For more information and to have your say, see our website.

Read More

ANZ Food Standards Code, 24-05-23

https://mailchi.mp/ef6438295cef/food-standard-news-1300748

Modified SDMT for the recalculation of buffer zones for products under PER93132

2023-05-23

The Australian Pesticides and Veterinary Medicines Authority (APVMA) has released a modified version of its Spray Drift Management Tool (SDMT) to allow for the recalculation of buffer zones for products authorised under PER93132.

PER93132, held by Grain Producers Australia, has been issued by the APVMA to allow applicators to access and use the modified SDMT for selected products in cereals and fallow situations.

Rather than simply applying the 'worst case' buffers when planning their spraying programme, applicators can now input site-specific information into the modified SDMT and calculate reduced buffer zones applicable to their local conditions, application preferences, and drift reduction technology.

In addition to the benefit of buffer zone reductions, use of the modified SDMT will allow users to recalculate buffer zones, reducing the need to provide a wide range of application options on the label. The modified SDMT is also intended to increase applicator understanding of the relationship between application parameters and off-target drift.

More information about the modified SDMT and PER93132 is available on our website.

Read More

APVMA, 22-05-23

https://apvma.gov.au/node/113416

Review of guidelines for determining a minor use

2023-05-04

The Australian Pesticides and Veterinary Medicines Authority (APVMA) is reviewing its guidelines for determining a minor use, to ensure they remain fit for purpose in a modern regulatory environment.

Minor use permits are issued by the APVMA to allow for the legal use of agricultural and veterinary chemicals in situations where registration of the product would not produce sufficient economic return.

The APVMA has developed guidance to assist applicants in determining whether a particular use can be defined as a minor use. These guidelines were first developed in the early 2000s and have since received minimal updates. As the agricultural landscape has changed over time, crops that were once considered major may now command only a small market share, whereas previously minor crops may have seen a surge in popularity or value.

The APVMA is seeking public feedback on the guidance in its current form and input into factors that should be considered during the update. The closing date for submissions is 15 June 2023. More information on how you can make a submission is available on the APVMA website.

Once the new guidelines are developed, there will be a second round of public consultation and the APVMA will seek feedback on the new guidelines.

Questions about the project can be directed to enquiries@apvma.gov.au.

Read More

APVMA, 04-05-23

https://apvma.gov.au/node/112466

Chinese government and industry work on FCM regulation

2023-05-25

China amending the national food contact material (FCM) regulation for the first time since 2016; amendments would expand use of previously approved food contact chemicals (FCCs) and food additives; redefines FCM to clarify that packaging material must contact the food item; industry association issues draft guidance; regulatory agencies approve or in process of approving multiple new FCCs

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The Government of China is updating the General Safety Requirements for Food Contact Materials and Articles (GB 4806.1), which is the primary legislation for the regulation of food contact materials (FCMs) in the country. Additionally, in recent weeks, new substances have been added to the positive list for FCMs and the allowed uses of other substances was expanded.

FCM regulation amendments

According to reporting from Chemical Watch, the National Center for Food Safety Risk Assessment (CFSA) "plans to expand the scope" of GB 4806.1 to incorporate polymers, broader uses of previously approved materials, as well as food ingredients. In the update, plastics, rubber, silica gel, paints, adhesives, and oil paints, that already have CFSA approval could be blended for use in FCMs, provided no chemical reactions occur. This revision also permits substances approved as food ingredients, like preservatives, to be utilized in FCM manufacturing, contingent on meeting GB 4806.1 requirements. Other amendments define the terms 'complete barrier layer', redefine 'effective barrier layer', and explicitly exclude outer packaging or material from the 'food contact material' definition unless it directly contacts food.

Voluntary industry standards

Website Packaging Law reports that the China National Food Industry Association published two new voluntary standards in February 2023 that build on top of the regulations included in GB 4806.1. China's national FCM standard includes general regulations, but when writing a Declaration of Compliance companies may need more guidance. The two voluntary industry standards cover declarations for FCMs/FCAs and adhesives, T/CNFIA 162-2022, and T/CNFIA 163-2022, respectively. The association plans to develop a voluntary standard for printing inks as well.

Read More

FPF, 25-05-23

https://www.foodpackagingforum.org/news/chinese-government-and-industry-work-on-fcm-regulation

AMERICA

Ditch sunscreens with "troublesome" oxybenzone, experts say

2023-05-2023

Oxybenzone, a UV-absorbing chemical that harms coral reefs and may impact the body's hormonal system, is found in 6% of sunscreens on the market in the U.S. this year, according to the Environmental Working Group's (EWG) annual sunscreen trends report.

Use of oxybenzone has declined by more than half since 2022, when it was present in 15% of products.

Sunscreen plays a crucial role in preventing health harms from sun exposure, such as skin cancers, but experts say it's important to evaluate ingredients to ensure they aren't creating new health risks. Indications that oxybenzone could affect the body's hormonal system has led to calls for its removal from sunscreens. In addition, some sunscreens fail to achieve their stated SPF (sun protection factor) rating. Many don't protect against UVA radiation, a part of the light spectrum that doesn't cause sunburns but can cause skin cancers. Advocates say the sunscreen market needs reform to provide the safest and most effective products to consumers.

Read More

EHN, 23-05-23

https://www.ehn.org/reef-safe-suncreen-2660532235.html

Regulatory Developments: Canada Begins Public Consultation on Draft State of PFAS Report, Proposes to Recommend Adding PFAS to CEPA Schedule 1

2023-05-24

On May 20, 2023, Canada published a Canada Gazette notice announcing the availability of its Draft State of Per- and Polyfluoroalkyl Substances (PFAS) Report (Draft Report). Canada proposes to conclude that the class of PFAS meets one or more criteria set out in Section 64 of the Canadian Environmental Protection Act, 1999 (CEPA). According to the notice, the Minister of the Environment and the Minister of Health (the ministers) propose to recommend that the class of PFAS be added to the CEPA Schedule 1 List of Toxic Substances. The Draft Report provides a qualitative assessment of the fate, sources, occurrence, and potential impacts of

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PFAS on the environment and human health to inform decision-making on PFAS in Canada. The ministers have released a risk management scope document for PFAS to initiate discussions with stakeholders on the development of risk management options. Comments on the Draft Report and risk management scope document are due July 19, 2023.

Draft Report

According to the Draft Report, the common chemical characteristic of PFAS is their perfluoroalkyl moiety, "which is extremely stable in the environment, to the extent that PFAS have often been termed 'forever chemicals.'" The Draft Report states that simple PFAS are highly persistent, whereas more complex molecules transform into stable PFAS. In the Draft Report, the term PFAS refers to the Organization for Economic Cooperation and Development's (OECD) broad chemical definition, "which -- with a few noted exceptions -- includes any chemical with at least a perfluorinated methyl group (–CF3) or a perfluorinated methylene group (–CF2–)." The Draft Report notes that this definition "captures substances with a wide range of structures and properties, from discrete chemicals such as perfluorocarboxylic acids, perfluorosulfonic acids, and fluorotelomer alcohols, to side-chain fluorinated polymers and high molecular weight fluoropolymers." Some PFAS on the market also possess structural attributes other than perfluoroalkyl chains (e.g., inclusion of ether linkages or chlorine atoms in the fluorinated hydrocarbon chains).

The Draft Report states that typical uses of PFAS include surfactants, lubricants, and repellents (for dirt, water, and grease). PFAS can also be found in certain firefighting foams (i.e., aqueous film-forming foams (AFFF)), textiles (e.g., carpets, furniture, and clothing), cosmetics, and food packaging materials.

According to the Draft Report, there are many potential sources of PFAS in Canada that can lead to human exposure and releases to the environment. Humans can be exposed to PFAS from various sources such as food and food packaging, cosmetics, products available to consumers, ambient air, indoor air and dust, and drinking water. The Draft Report states that PFAS-impacted contaminated sites represent "hot spot" areas where Canadians and the environment may be exposed to elevated concentrations of PFAS. Such sites include those associated with the use of AFFFs. The Draft Report notes that as it is not possible to separate PFAS-containing waste from the general waste stream, PFAS-containing products can be found in municipal solid waste (MSW) landfills or are destined for MSW incineration. Composting of PFAS-containing food packaging, releases into wastewater

treatment systems, and the application of biosolids to land provide additional routes of entry for PFAS into the environment. The Draft Report states that "[i]t should be noted that PFAS contamination is present throughout Canada and is not limited to a few sources or areas."

Read More

Lexology, 24-05-23

https://www.lexology.com/library/detail.aspx?g=8f243e31-0f04-465b-9cd9-1c0283e73949

Michigan PFAS Drinking Water Challenge Briefing Complete

2023-05-26

We previously wrote regarding a Michigan state court ruling that struck down Michigan's PFAS regulations related to drinking water enforceable limits, with the ensuing appeal in December 2022 by the state. The state filed its legal brief at the end of February 2023 with the Michigan Court of Appeals, advancing several arguments of note. On May 15, 2023, the state filed its Reply brief on the issue. The significance of the Michigan PFAS challenge is that the arguments and lower court ruling provide clues as to similar arguments that we predict will be advanced when certain companies challenge federal drinking water standards and the CERCLA PFAS designation in courts.

Michigan PFAS Challenge

Michigan recently enacted PFAS drinking water standards for seven types of PFAS – PFOA (8ppt), PFOS (16ppt), PFNA (6ppt), PFHxA (400,000ppt), PFHxS (51ppt), PFBS (420 ppt) and the Gen-X chemical HFPO-DA (370 ppt). 3M challenged the regulations in court on three grounds: (1) Michigan had not shown that the standards were necessary, (2) the standards were enacted in a manner such that they were arbitrary and capricious, and (3) there were deficiencies in the state's regulatory-impact statement (a required part of the regulatory process). The Court dismissed the first two arguments; however, it found in favor of 3M on the third ground. In short, the Court found that Michigan had not properly considered the cost impacts of the standards to companies and so the impact statement that was written was faulty.

While the ruling technically does strike down the Michigan regulations, the Court also ruled that it would stay its decision and not make it effective

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until final judgment is entered. As such, the Michigan PFAS regulations will remain in effect during the period of time when the current appeal is pending. The Court also made note that the entire lawsuit and the drinking water standards could be moot if the EPA's drinking water standards are ultimately more aggressive than Michigan's.

Read More

The National Law Review, 26-05-23

https://www.natlawreview.com/article/michigan-pfas-drinking-water-challenge-briefing-complete

'This Is the First Step': Minnesota Passes Most Comprehensive PFAS Ban in the Nation

2023-05-26

Minnesota Gov. Tim Walz on Wednesday signed into law the broadest ban on dangerous "forever chemicals" in the nation.

The ban forms part of H.F. 2310—an omnibus environment bill—and is one of the many new policies to come out of what progressives say is a "transformational" legislative session for the state. Minnesota is now the first of any U.S. state to prohibit per- and polyfluorinated substances (PFAS) in menstrual products, dental floss, cleaning supplies, and cooking equipment.

"Minnesota is at the forefront of addressing the PFAS and toxic chemical crisis," Safer States national director Sarah Doll said in a statement. "This law shows that states are a key part of ensuring that communities are safe from PFAS."

PFAS are a class of chemicals that have been used by industry since the 1940s. They are common in firefighting foam and stick-, stain-, grease-, and water-resistant products. However, they have spread extensively throughout the environment and human bodies where they do not break down—hence the moniker "forever chemicals." This is a problem because they have also been linked to an expanding list of health concerns including cancer, immune suppression, reproductive and developmental issues, and thyroid and liver ailments.

Read More

Common Dreams, 26-05-23

https://www.commondreams.org/news/minnesota-passes-nation-s-most-comprehensive-pfas-ban

EUROPE

France needs to invest €66bn a year on climate action, government report states

2023-05-24

France Stratégie, an advisory body attached to the Prime Minister's office, published its report Monday (22 May) on the economic costs of meeting the objectives of the Paris Agreement on climate change.

"This report will be a landmark in the economics of climate change. Like the Meadows report," Industry Minister Roland Lescure told EURACTIV France. The Meadows report, published in 1972, was the first to theorise the limits to economic growth in the context of climate change.

According to the report, climate action will cost France more than €66 billion annually until 2030. Of that sum, €48 billion will have to be spent on renovating buildings – whether business, residential or public. Another €7 billion a year will have to be invested in the energy field, while €3 billion a year will need to be spent on road transport.

The catch, however, is that a large part of these investments will have to be provided by households, the report notes. Switching to an electric car and renovating the home, for example, come at a price tag which is worth one year of salary for middle-class households and two years of salary for many others in the lower income bracket.

"If we do not work on the issue of social justice in this transition, we will go from failure to renunciation", said Cécile Duflot, a former minister now director of Oxfam France who was invited to the report's presentation on Wednesday (24 May).

To do this, it will be necessary to finance the transition through public finances, to the tune of €25-34 billion annually, the report says.

Read More

Euractiv, 24-05-23

https://www.euractiv.com/section/energy-environment/news/france-needs-to-invest-e66bn-a-year-on-climate-action-government-report-states/

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Toxic chemical combinations found at over 1,600 river and groundwater sites across England

2023-05-24

New analysis of Environment Agency data appears to reveal a worrying level of chemical pollution in rivers and other freshwater sites across England.1 The research, which looked at the prevalence of five "chemical cocktails" known to have toxic impacts for wildlife, also highlights the lack of official monitoring for known harmful chemical cocktails, as well as the lack of a regulatory framework to address these mixtures.

Findings from Wildlife and Countryside Link and The Rivers Trust reveal that:

- Chemical cocktails, that have been proven harmful to wildlife in scientific studies, have been found in 814 river and lake sites (out of 1,006 sites with data – 81%) and 805 groundwater sites (out of 1,086 sites with data – 74%) across England
- Over half (54%) of these sites contained 3 or more of the 5 harmful chemical cocktails investigated2
- Up to 101 chemicals were identified in river samples, with sites along the rivers Mersey, Stour, Colne, Thames, Trent, Yare, Irwell, Medway, Humber and Avon among those containing the highest numbers of chemicals. The actual numbers of chemical pollutants will be even higher3

The chemical cocktails found across the 1,619 sites contained six different chemicals in five different hazardous mixtures. These included four toxic forever chemicals PFOS, PFOA, PFBS and PFHxS, the pesticide 2,4-D and the commonly used painkiller ibuprofen (see table below for more detail). In specific combinations these chemicals are known to have increased harmful impacts on a range of species including amphibians, fish, insects, nitrogen-fixing bacteria and algae. Identified detrimental effects included reduced growth, cell function, impacts on embryos and lower survival rates. Any potential human health implications, for example through contact via bathing or recreation, remain unknown.

Read More

Envirotec, 24-05-23

https://envirotecmagazine.com/2023/05/25/toxic-chemical-cocktails-found-at-over-1600-river-and-groundwater-sites-across-england/

Ukraine aligns with EU packaging and chemical regulations

2023-05-23

The Ukrainian government has made several announcements through spring 2023 that it is adopting new regulations to align the country with the European Union's Classification, Labelling and Packaging (CLP) Regulation as well as the Packaging and Packaging Waste Regulation.

According to the Ministry of Environmental Protection and Natural Resources, most components of the Ukrainian CLP regulation will enter into force on July 9, 2023. A few components such as identifiers of dangerous chemical products and packaging are not being implemented until June 29, 2024.

A separate draft law aims to regulate packaging and packaging waste in Ukraine, introducing new norms and requirements to reduce hazardous substances in packaging, establishing Extended Producer Responsibility Organizations, and setting recycling targets. The law is planned to come into effect on January 1, 2024, with specific provisions entering into force in stages until January 1, 2027. These specific provisions include the phase-out of non-compliant packaging that was on the market prior to the implementation of the regulation and the application of fines to non-compliant companies.

The country has been working towards harmonizing its legislation with the EU since becoming an EU candidate in 2022 (FPF reported.

Read More

FPF, 23-05-23

https://www.foodpackagingforum.org/news/ukraine-aligns-with-eu-packaging-and-chemical-regulations

Experts convene for Chemical Weapons Demilitarisation Conference

2023-05-23

- More than 99% of declared chemical weapons stockpiles destroyed to date
- International experts meet to address remaining chemical weapons challenges

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Scientists, technical experts, policy officials and non-governmental organisations from across the world congregated at the 25th Chemical Weapons Demilitarisation Conference in London to share experiences and lessons and address remaining challenges.

The Conference has been hosted by the Ministry of Defence and Defence Science and Technology Laboratory (Dstl), in close collaboration with the U.S. Department of Defense. The annual conference is crucial to facilitating conversations on the demilitarisation of chemical weapons.

As more than 99% of declared chemical weapons stockpiles have been destroyed, and with the remainder scheduled to be destroyed this year, this year's conference addressed the future of demilitarisation. Speakers expanded the remit by presenting on topics such as biotoxins and the capability of states not party to the Chemical Weapons Convention.

Delivering the closing remarks of the Conference, UK Defence Minister Baroness Goldie reflected on key successes, such as 72,000 metric tonnes of the declared chemical warfare agents across the world being verifiably destroyed – as well as condemning those who have used and retained chemical weapons – acknowledging the importance of holding those responsible to account.

Read More

Gov.uk, 25-05-23

https://www.gov.uk/government/news/experts-convene-for-chemical-weapons-demilitarisation-conference

EFPIA and ECHA publish more data to help developing alternative methods to animal tests

2023-05-17

Additional information about the hazard properties of 75 substances from 370 tests has recently been published as IUCLID datasets. This more than doubles the amount of data that was made initially available for the scientific community developing alternative test methods when the joint initiative kicked off a year ago.

Helsinki, 17 May 2023 – A pilot project led by the European Federation of Pharmaceutical Industries and Associations (EFPIA), and supported by ECHA, has made an updated set of archived data from unpublished chemical tests available on the IUCLID website. The database contains now altogether information about the hazard properties of 94 substances from 517 tests. This follows the project's initial delivery of data one year ago.

This data can help, for example, to develop predictive computational testing models, read across and other alternative test methods with the objective to decrease the reliance on animal testing. The following table gives an overview of the number and type of studies by endpoint groups.

Read More

ECHA, 17-05-23

https://echa.europa.eu/-/efpia-and-echa-publish-more-data-to-help-developing-alternative-methods-to-animal-tests

Understanding the Drinking Water Directive

2023-05-2

The revised Drinking Water Directive (DWD) aims to protect citizens and the environment from the harmful effects of contaminated drinking water and to improve access to drinking water. It came into force on 12 January 2021 following a review of the original Drinking Water Directive of 1998.

The directive introduces minimum requirements for materials that are in contact with water intended for human consumption throughout the EU. This harmonisation contributes to reaching a uniform level of protection of health for all EU citizens and improves the functioning of the internal market.

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Article 11 of the revised directive sets out the framework for minimum hygiene requirements for materials in contact with drinking water. ECHA will support the European Commission in this work by preparing:

- European positive lists of starting substances, compositions and constituents that are authorised for use in the manufacture of materials in contact with drinking water.
- Risk assessment methodologies and information requirements for reviewing starting substances, compositions and constituents that could be added to the positive lists.
- Administrative procedures for updating the positive lists.
  After the positive lists are published, ECHA will continue keeping the lists up to date, by adding new entries and amending or removing existing entries.

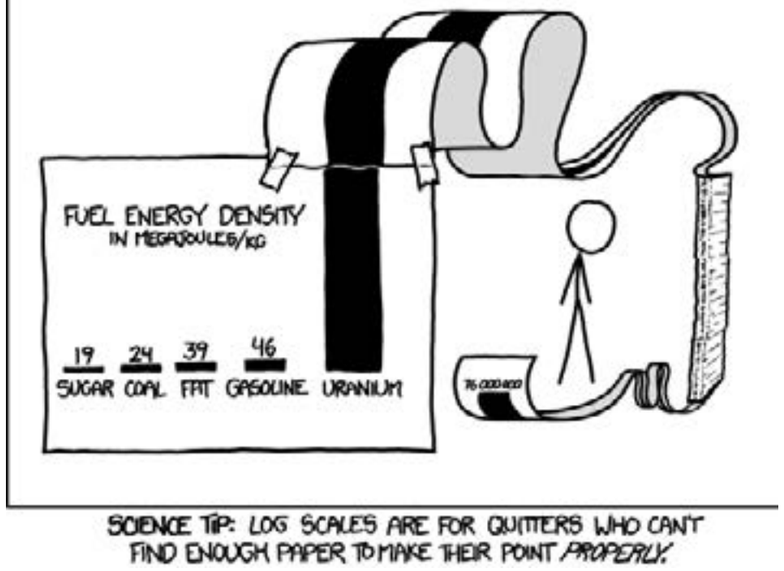
Read More

ECHA, 24-05-23

https://echa.europa.eu/understanding-dwd

Log Scale

2023-05-31



(https://xkcd.com/1162/)

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Isopropyl Alcohol

2023-06-02

Uses [1,3]

Isopropyl alcohol is used across a range of applications. It is primarily used as a solvent and in the medical industry as a cleaning agent. As a solvent it is used in many home cleaning products, as its ability to evaporate quickly means there is little chance of shock or damage to electrical components. In the medical industry, isopropyl alcohol is commonly used as an ingredient in rubbing alcohol, with distilled water. It is also used in disinfecting pads. In addition, isopropyl alcohol is used as an ingredient in a range of products, including make soaps, window cleaners, antifreezes, perfumes and more.

Routes of Exposure [1]

Pure isopropyl alcohol is readily absorbed through the skin.

Home-use products with isopropyl alcohol in them usually have approximately 70% of the compound in them, so they are less toxic than industry-standard versions. However, there is still a chance of toxic exposure.

Health Effects

Isopropyl alcohol poisoning affects a range of systems, including the nervous and respiratory systems.

Acute Effects [1,5]

Severity of symptoms depend on the level and type of exposure.

Acute exposure to the chemical compound can result in headaches, vomiting, dizziness, nausea, unconsciousness, comas, and death. Exposure can also cause CNS depression, low arterial pressure, abdominal pain, slowing respiration and coughing.

Chronic Effects [1,5]

Chronic exposure to isopropyl alcohol is toxic to multiple body systems. Long term exposure to the chemical compound can cause cracking, red, itchy and dry skin; impaired memory and inflammation of the skin. There is not a glut of information regarding long term exposure to isopropyl alcohol specifically, but generally, chronic exposure to solvents is known to increase the risk of kidney and liver dysfunction.

Isopropyl alcohol (aka isopropanol) is a colourless, combustible liquid with a strong odour. Its chemical formula is CH3CHOHCH3. Isopropyl alcohol is a volatile liquid, and if left exposed to the elements, it will evaporate quickly. [1,2,3]

Safety

First Aid Measures [5]

Ingestion: DO NOT INDUCED VOMITING. Rinse victim's mouth with water. Get immediate medical attention.

Skin contact: Remove all contaminated clothing, footwear and accessories. Do not re-wear clothing until it has been thoroughly decontaminated. Immediately rinse affected areas with plenty of water. If symptoms persist, contact a doctor immediately.

Eye contact: Flush eyes (including under the eyelids), with water for at least 15 minutes. Contact a medical professional.

Inhalation: Take victim to the nearest fresh air source and monitor their breathing. Keep the victim warm. If the victim is not breathing, and you are qualified, you may perform CPR with a one-way valve or protective mask. Immediately contact a medical professional.

General: Never administer anything by mouth to an unconscious, exposed person.

Exposure Controls/Personal Protection [4]
Engineering controls: Emergency eyewash fountains and quick-drench areas should be accessible in the immediate area of the potential exposure. Ensure there is adequate ventilation. Use a local exhaust ventilation or process enclosure, to limit the amount of acid in the air.

Personal protection: Safety glasses, protective and dustproof clothing, gloves, an apron and an appropriate mask or dusk respirator. Wear impervious shoes. Do not wear contact lenses. For specifications regarding other PPE, Follow the guidelines set in your jurisdiction.

Regulation [6]

United States:

The Occupational Safety and Health Administration (OSHA) has set an 8-hour time weighted average (TWA) concentration limit for isopropyl alcohol of 400ppm.

Australia [5]

An 8-hour TWA for isopropyl alcohol of 400ppm has been set.

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Taking carbon dioxide from the atmosphere and turning it into vinegar

2023-05-30

The Australian, US, and Japanese researchers, who published their research in Nature Communications, say their method points to a scalable way to turn carbon dioxide emissions into useful materials.

There's worldwide demand for about 6.5 million tonnes of acetic acid each year, to make a range of products including pharmaceuticals, vinyls, textiles, and cosmetics.

It's also the main component of vinegar, and is often used as a food preservative.

In the food industry, acetic acid is mostly made by fermenting, but in other industries it's made from fossil fuels, releasing greenhouse gas emissions in the process. The production typically also needs expensive precious metals like cobalt, iridium and rhodium to work.

Now this team has figured out how to make acetic acid from carbon dioxide and hydrogen, using (cheaper) iron as a catalyst.

The iron catalyst also stays solid for the entire reaction, meaning the process doesn't need extra equipment and energy to purify the acetic acid once it's made.

"From theory we knew iron should be a good candidate for catalysing this reaction, but the challenge is to keep it stable under acidic water conditions," says senior author Associate Professor Akshat Tanksale, a chemical engineer at Monash University.

Making acetic acid produces – unsurprisingly – acid dissolved in water.

"As is commonly known, iron rusts – oxidises – in water, whereas we wanted it to remain at least partially in the metallic form," says Tanksale.

The researchers' solution was to use a metal-organic framework (MOF): a substance made from metallic atoms (in this case, iron), linked with carbon-based bridges, forming a sort of sponge with molecule-sized holes in it.

They then heated the MOF, allowing some of the iron atoms to fuse together and form particles a few nanometres in size, embedded in a porous layer of carbon.

Researchers have made a catalyst that can turn carbon dioxide into acetic acid, a tremendously useful industrial chemical and food additive.

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Diagram of neatly organised large molecule breaking into more disordered molecule with large green blobs indicating iron

Thermal transformation – heating something in a controlled environment – can convert this substance called at MOF into a catalyst for turning CO2 into acetic acid. Credit: Supplied by Monash University

The resulting catalyst could make acetic acid (CH3COOH) out of CO2 and hydrogen (H2) very efficiently.

Tanksale says that it took his team more than a year, with some trial and error, to land on this catalyst.

"We started working on this project at the start of COVID-19 pandemic in 2020, so my research staff and students weren't allowed in the lab every day and they had to work alone in shift rotations," he says.

"It took us another 18 months to provide definitive evidence for how this catalyst works at the molecular level, while having to deal with a number of lockdown periods in Melbourne."

The catalyst is cheaper than those currently used, and the researchers are working on commercialising it.

The bottleneck, says Tanksale, is not the catalyst itself but the feedstocks: CO2 and hydrogen.

"While they are readily available today, their cost is significantly higher if it is derived from green sources," he says.

"To reap the true benefits of our technology, i.e. to achieve negative carbon emissions, carbon dioxide must be captured from air, and hydrogen must be made from water using renewable energy (green hydrogen).

"These enabling technologies are yet to reach their full commercial potential."

cosmosmagazine.com, date

https://cosmosmagazine.com

Using AI to create better, more potent medicines

2023-05-30

Today, most drug discovery is carried out by human chemists who rely on their knowledge and experience to select and synthesize the right

While it can take years for the pharmaceutical industry to create medicines capable of treating or curing human disease, a new study suggests that using generative artificial intelligence could vastly accelerate the drug-development process.

molecules needed to become the safe and efficient medicines we depend on. To identify the synthesis paths, scientists often employ a technique called retrosynthesis—a method for creating potential drugs by working backward from the wanted molecules and searching for chemical reactions to make them.

Yet because sifting through millions of potential chemical reactions can be an extremely challenging and time-consuming endeavor, researchers at The Ohio State University have created an AI framework called G2Retro to automatically generate reactions for any given molecule. The new study showed that compared to current manual-planning methods, the framework was able to cover an enormous range of possible chemical reactions as well as accurately and quickly discern which reactions might work best to create a given drug molecule.

"Using AI for things critical to saving human lives, such as medicine, is what we really want to focus on," said Xia Ning, lead author of the study and an associate professor of computer science and engineering at Ohio State. "Our aim was to use AI to accelerate the drug design process, and we found that it not only saves researchers time and money but provides drug candidates that may have much better properties than any molecules that exist in nature."

This study builds on previous research of Ning's where her team developed a method named Modof that was able to generate molecule structures that exhibited desired properties better than any existing molecules. "Now the question becomes how to make such generated molecules, and that is where this new study shines," said Ning, also an associate professor of biomedical informatics in the College of Medicine.

The study was published today in the journal Communications Chemistry.

Ning's team trained G2Retro on a dataset that contains 40,000 chemical reactions collected between 1976 and 2016. The framework "learns" from graph-based representations of given molecules, and uses deep neural networks to generate possible reactant structures that could be used to synthesize them. Its generative power is so impressive that, according to Ning, once given a molecule, G2Retro could come up with hundreds of new reaction predictions in only a few minutes.

"Our generative AI method G2Retro is able to supply multiple different synthesis routes and options, as well as a way to rank different options for each molecule," said Ning. "This is not going to replace current lab-based

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experiments, but it will offer more and better drug options so experiments can be prioritized and focused much faster."

To further test the AI's effectiveness, Ning's team conducted a case study to see if G2Retro could accurately predict four newly released drugs already in circulation: Mitapivat, a medication used to treat hemolytic anemia; Tapinarof, which is used to treat various skin diseases; Mavacamten, a drug to treat systemic heart failure; and Oteseconazole, used to treat fungal infections in females. G2Retro was able to correctly generate exactly the same patented synthesis routes for these medicines, and provided alternative synthesis routes that are also feasible and synthetically useful, Ning said.

Having such a dynamic and effective device at scientists' disposal could enable the industry to manufacture stronger drugs at a quicker pace—but despite the edge AI might give scientists inside the lab, Ning emphasizes the medicines G2Retro or any generative AI creates still need to be validated—a process that involves the created molecules being tested in animal models and later in human trials.

"We are very excited about generative AI for medicine, and we are dedicated to using AI responsibly to improve human health," said Ning.

phys.org, 30 May 2023

https://phys.org

Colour-changing microcrystals could be a cheap and safe way to monitor medicines

2023-06-01

It's a feature that could become very useful in tracking medicines.

It can be frustrating to figure out whether the food inside it is still safe to eat if a power outage stops your fridge from working for a few hours – maybe some food at the back stayed cool enough to avoid spoilage, but maybe it didn't.

This problem is much, much more concerning when industrial fridges and freezers, carrying commercial amounts of food – or medicines – break down.

It's possible to track the temperature of packs of vaccines with monitors – but these are either expensive electronics or flawed in design.

A team of Chinese and US researchers has invented a class of microcrystal that changes colour dramatically as the temperature changes.

Commercially available substances that change colour with the temperature tend to fade, and they're mostly designed to spot whether something gets above 0°C. This is still too warm for things like the Pfizer and Moderna COVID-19 vaccines, which need to be kept at −70 °C and −20 °C, respectively.

New research published in ACS Nano has suggested an alternative, demonstrating materials with robust colour changes that can be tuned to specific temperatures.

The materials are made from tiny grains of silica, each a few hundred nanometres in size: nanoparticles coated with glycerol.

These nanoparticles exhibit structural colour: waves of light bounce off them in a way that makes them gleam in bright reds and greens, like the wings on beetles.

The researchers combined these microcrystals with mixtures of water and ethylene or polyethylene glycol, which melt at different temperatures depending on the different proportions of each chemical.

When the brightly coloured mixtures became hot enough to melt, the microcrystals broke open and all the structural colour vanished, leaving a dull colourless substance.

This wasn't reversible: even if the mixture froze again, the colour was gone.

The researchers were able to tune their mixtures to change colour at any point between -70°C and 37°C, and to demonstrate their efficacy used these substances to print both a QR code for monitoring temperature history on a "donated" organ (using a model pig's heart) and flexible labels that could go on top of vaccine vials.

In both cases, the systems were very sensitive, and signalled clearly when temperatures became too warm.

In their paper, the researchers write that their materials "have established a general design rule for next-generation intelligent indicators, holding promise for reliable cold chains".

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"In addition, we anticipate that structural colour liquids will benefit various areas such as wearable sensors, droplet robots, and photonic display," they add.

cosmosmagazine.com, 01 June 2023

https://cosmosmagazine.com

With a zap of electricity, recyclable (and recycling) polymers can form

2023-05-22

The team, from Flinders University, has tapped into the concept of 'electrochemistry' to develop a simple and quick reaction to make their polymers.

The reaction can be done at room temperature, with no additional ingredients – meaning it doesn't need extra energy or hazardous chemicals.

They've published their method in the Journal of the American Chemical Society.

The reaction begins with a low-cost substance called a "trisulphide": an organic (carbon-containing) molecule with three sulphur atoms in it.

When an electron is added via electricity, the sulphur atoms in one molecule bind to sulphur atoms in another, setting up a systematic chain reaction.

This forms a polytrisulphide: a long molecule made up of repeating units, linked together with sulphur atoms.

This sulphur polymer can bind to precious metals, like gold. The researchers tested it out on mixtures that resembled ones produced in gold mining and e-waste recycling, and found it could remove 97% of the gold.

"The use of electricity to produce new materials is an emerging field of research that opens many doors to new chemicals and polymers that can be produced in a more sustainable way," says co-author Dr Thomas Nicholls.

Co-author Professor Justin Chalker says that while electrochemistry has been used for a while in metal refining, battery technologies, future fuels

A little electricity has helped a team of chemists to make sustainable polymers that could improve e-waste recycling, precious metal mining and perhaps even work as antimicrobials.

like hydrogen, and making disinfectants like chlorine, using it to make complex molecules like this polymer is a relatively new field.

"The interest is growing because only electricity is needed to provoke the key reactions, and they can be tuned to react selectively at different parts of the molecules. In our case, this selectivity allowed a unique way to make a recyclable polymer," says Chalker.

The polymer is recyclable because it can easily be converted back into its single-molecule building blocks, ready to use again.

"Our method to electrochemically produce polymers provides new materials that are highly functional and environmentally friendly," says first author Jasmine Pople, a PhD candidate at Flinders.

Pople adds that the method "may generate less waste than traditional chemical syntheses, and it can be powered with renewable energy".

With some quantum mechanical calculations, the team was able to figure out exactly how their polymer grew.

"The polymerisation has a clever self-correcting mechanism: whenever the wrong reaction occurs, it reverses until the correct reaction proceeds, ensuring a uniform polymer," says co-author Dr Le Nhan Pham.

Next, the team is planning to see what other polymers they can make with this technique.

"There are a variety of new structures and functions we want to build into these polymers," says Chalker.

"We also have plans to broaden the length of the polymer chains to improve their mechanical properties.

"With new functional groups, we envision applications in biochemistry, sustainable construction, battery technologies, smart coatings and more."

cosmosmagazine.com, 22 May 2023

https://cosmosmagazine.com

The device you're currently reading this story on needs tiny chunks of metals like neodymium and dysprosium to work.

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Protein can sort rare earth elements better than current mining practices

2023-06-01

So do wind turbines, electric vehicles and lasers.

These rare earth elements are vital to modern technology, but they're hard to mine and recycle because they're tricky to distinguish from each other.

Now, a team of US researchers has engineered a protein that sorts rare earth elements quickly and without any of the extra energy or noxious chemicals currently used industrially.

Their findings are published in Nature.

"Biology manages to differentiate rare earths from all the other metals out there — and now, we can see how it even differentiates between the rare earths it finds useful and the ones it doesn't," says lead author Associate Professor Joseph Cotruvo Jr., a chemist at Penn State University, US.

"We're showing how we can adapt these approaches for rare earth recovery and separation."

The protein specifically focuses on lanthanides: the class of 15 elements following lanthanum in the periodic table.

Lanthanides are relatively abundant in the Earth's crust – but they're mostly present in low concentrations.

They all have similar atomic sizes and chemical properties, which makes them very hard to separate.

Separating lanthanides needs dozens, sometimes hundreds, of reactions, using substances that can be quite toxic, like kerosene and phosphonates.

"This is the biggest and most interesting challenge, discriminating between the individual rare earths, because they are so alike," says Cotruvo.

"We've taken a natural protein, which we call lanmodulin or LanM, and engineered it to do just that."

The researchers first isolated lanmodulin in 2018, from a type of bacteria called a "methylotroph".

They showed that the protein could separate lanthanides from other metals but was less effective at distinguishing them from each other.

The researchers went looking for similar proteins that might more discerning properties. They landed on a protein from the bacterium Hansschlegelia quercus, which they'd isolated from English oak buds.

This protein could distinguish between lighter and heavier lanthanides.

"This was surprising because these metals are very similar in size," says Cotruvo.

"This protein has the ability to differentiate at a scale that is unimaginable to most of us — a few trillionths of a metre, a difference that is less than a tenth of the diameter of an atom."

It does this by pairing up. In the presence of lighter lanthanides, the protein "dimerises": two proteins bind together to form a bigger molecule called a dimer. When it gets to heavier lanthanides, the pairing is much less strong.

The researchers used X-ray crystallography to determine which part of the protein was performing this function.

With this data, they were able to use the protein to separate out neodymium and dysprosium, two key smartphone magnet components, at room temperature with just one step.

"While we are by no means the first scientists to recognise that metal-sensitive dimerisation could be a way of separating very similar metals, mostly with synthetic molecules, this is the first time that this phenomenon has been observed in nature with the lanthanides," says Cotruvo.

The protein still lacks some finesse. It can sort the lightest lanthanides from the heaviest, but it can't yet distinguish between lanthanides that are close in size.

For instance, sorting neodymium (atomic number 60) from its next-door neighbour praseodymium (59) isn't yet possible.

Cotruvo calls this the "toughest problem of all", but thinks that with further optimisation it "may be within reach".

The team has filed a patent application for the process and is now looking to commercialise it.

cosmosmagazine.com, date

https://cosmosmagazine.com

Legislation under consideration by the Italian government would prohibit the production, export or import of synthetic 'meat' grown from animal cells. If approved, the bill would introduce a fine of €10,000–€60,000 (£8800–£53,000) for any violation of the proposed ban, which would reportedly include other food and drink products similarly derived from cells in a laboratory, several media outlets including Reuters reported.

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Italian government considers banning lab-grown meat

2023-05-05

'The passing of such a law would shut down the economic potential of this nascent field in Italy, holding back scientific progress and climate mitigation efforts, and limiting consumer choice,' warned Alice Ravenscroft, head of policy at the Good Food Institute Europe. It could prevent Italian scientists from pursing this field and put an end to cultivated meat startups in the country, she added.

'The EU already has a robust regulatory process in place for confirming the safety of new foods like cultivated meat, and regulators in the United States and Singapore have already found it to be safe,' Ravenscroft added. This development puts Italy at odds with the rest of Europe, she suggested, noting that the Netherlands last year announced €60 million in government funding to support cellular agriculture, and the UK government also putting up £16 million for sustainable novel food production systems in December 2022.

Cellular Agriculture Europe called the proposed law 'unnecessary' because food products can only enter the EU market if they are authorised by the European Commission, following a thorough safety assessment by the European Food Safety Authority.

'This ban could be damaging the economic opportunity for Italy and the EU to be at the forefront of this innovation, to contribute to strengthening Europe's food self-sufficiency in the face of fragile supply chains, increased domestic and international supply constraints and its competitiveness in the global agri-food industry,' cautioned Cellular Agriculture Europe, a coalition of companies dedicated to producing cell culture-based foods.

In November, the US Food and Drug Administration gave initial approval for cultivated meat to be sold in the US, declaring California-based Upside Foods' cultured chicken to be safe for consumption. Then in March, the agency gave Good Meat a 'no questions' letter indicating its acceptance of the company's conclusion that its cultivated chicken – sold in Singapore for more than two years – is also safe to eat.

The only company anywhere in the world that is currently permitted to sell cultured meat to consumers is Eat Just, which began doing so in Singapore in late 2020.

chemistryworld.com, date

https://chemistryworld.com

Look closely at a glass of champagne, and you'll notice that the bubbles stream upwards in organised single-file chains.

Why champagne bubbles are neater than beer or water bubbles

2023-05-04

But in a glass of carbonated water, the bubbles zoom up from many different directions, veering about as they do.

A group of US and French fluid mechanists have figured out why champagne forms these stable "bubble chains" when other bubbly drinks don't.

Their findings, published in Physical Review Fluids, could also be used to explain bubble flows in industrial processes.

"This is the type of research that I've been working out for years," says senior author Professor Roberto Zenit, an engineer at Brown University, US. "Most people have never seen an ocean seep or an aeration tank but most of them have had a soda, a beer or a glass of champagne. By talking about champagne and beer, our master plan is to make people understand that fluid mechanics is important in their daily lives."

The researchers investigated the bubbles in different fizzy beverages, including carbonated water, beer, champagne and some other sparkling wines. Champagne and sparkling wine have stable bubble chains, while the chains are only sometimes stable in beer and usually unstable in mineral water, making for much more random-looking bubbling.

The team filled a rectangular plexiglass container with each drink, then added a needle to the bottom to pump in gas and make their own, controlled bubbles in the drink.

They then either increased the bubble size of the gas bubbles they were pumping in, or added "surfactants" – substances that soften the border between two different fluids, like air and water. Surfactants are used as foaming agents in soaps and other bubbly products, and surfactant proteins appear naturally in champagne and beer.

"The theory is that in champagne these contaminants that act as surfactants are the good stuff," says Zenit.

"These protein molecules that give flavour and uniqueness to the liquid are what makes the bubble chains they produce stable."

The researchers found that adding surfactants could produce stable bubble chains in the unstable drinks.

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Confirming and explaining their results further with computer modelling, they believe that the surfactants in champagne let the bubbles leave smooth wakes, so the next bubble can rise easily in exactly the same path.

This explains why carbonated water, with no surfactants, tends to have unstable bubble chains.

"This wake, this velocity disturbance, causes the bubbles to be knocked out," says Zenit."Instead of having one line, the bubbles end up going up in more of a cone."

The researchers also found that blowing bigger bubbles could smooth much of this out, allowing for stable bubble chains without extra surfactants.

Aside from some nice pub trivia, the team say these results will be useful for other fluid mechanics problems.

For instance, they'll be relevant to examining carbon dioxide and methane vents on the ocean floor, and operating aeration tanks at water treatment plants.

"We're interested in how these bubbles move and their relationship to industrial applications and in nature," says Zenit.

cosmosmagazine.com, 4 May 2023

https://cosmosmagazine.com

A new, smarter method to detect IEDs

2023-05-25

Organic Peroxide Explosives (OPEs) are frequently used by terrorists, because they can be made from readily available materials and mixed in a domestic kitchen.

OPEs have been used in IEDs in terrorism events including the 2015 Paris attacks, the 2016 Brussels attacks, the 2017 Manchester bombing and the 2019 Sri Lanka bombings.

Swabs can pick up tiny traces of OPEs on skin, so it's possible to screen for people who've carried or made OPEs. This is often done at random in airports.

But the current screening method also picks up hydrogen peroxide, which is used in a variety of common household products including cleaning agents, hair dyes and nail polish removers.

An Australian team of researchers has developed a bet-ter way to screen people who might have been making improvised explosive devices (IEDs).

Research published in Analytica Chimica Acta has pointed to a new, more specific, technique, which avoids the problem caused by hydrogen peroxide, so could end up incorporated into standard airport and security screening.

"I was thinking that there should be a more portable, inexpensive and rapid screening method, which can be employed easily by anyone – it doesn't need to be a specialised or skilled person," says lead author Dr Parvez Mahbub, an adjunct fellow at Victoria University in Melbourne.

Mahbub and colleagues' technique uses chemiluminescence: molecules that glow when they react with certain chemicals.

After swabbing skin, the swabs are treated with a "miniscule" amount of sulphuric acid, which removes any hydrogen peroxide.

Then, a process called flow injection analysis with chemiluminescence detection allows the incriminating molecules in OPEs to show up.

"Within 15 seconds, we will have a result. So it is quite fast," says Mahbub.

So far, the researchers have showed that the process works when taking swabs from pig skin – a common analogue for human skin.

"To do it on humans, you need volunteers, as well as ethical clearance, as well as funding," says Mahbub.

His team is negotiating with funding agencies to continue the tests on people, as well as aiming to develop "version two" of the technology.

"I'm trying to replace acid with an advanced light source, for example LEDs, which might make it even more safe," says Mahbub.

This would convert the acid step into a simple button press. According to Mahbub, this will make the process more portable and faster, as well as safer.

The testing method is still some years away from widespread use, but Mahbub says that it's fast and simple enough that it could one day become a compulsory part of airport screening.

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"It will add some more extra functionality in terms of the ability to screen – because we would like to see which sample is coming from an explosive and which sample is just coming from a household product."

cosmosmagazine.com, 25 May 2023

https://cosmosmagazine.com

The old smallpox vaccine can protect against mpox

2023-04-25

The virus' spread (mostly among younger men who have sex with men) triggered a vaccine rollout with readily available vaccines.

Mpox vaccines are similar to the first modern vaccine: the smallpox vaccine. So similar, in fact, that a new study has found that old-school smallpox vaccination provides some protection against mpox.

The study, published in Cell Host & Microbe, looked at the "memory" cells (T-cells) in blood donors to see if those who were old enough to be vaccinated against smallpox were protected from mpox.

"Our study shows that this is the case, which implies that the memory cells are very long-lived and that they can recognise closely related viruses such as the mpox virus and provide overlapping, or cross-reactive immunity," says corresponding author Dr Marcus Buggert, a researcher at the Center for Infectious Medicine, at the Karolinska medical university in Sweden.

The researchers looked at blood from 105 healthy Swedish donors. Smallpox vaccination was compulsory in Sweden until 1976, when the program was ended because the disease was nearly eradicated (it was formally declared eradicated worldwide in 1980).

They found that blood from people born before 1976 had a significantly stronger immune response to both smallpox and mpox.

This means that their resistance to smallpox has lasted for decades, and that the vaccine can provide protection against other similar viruses.

Mpox vaccinations are available for at-risk groups in Australia.

cosmosmagazine.com, date

https://cosmosmagazine.com

Last year, mpox spread across the world for the first time, causing at least 85,000 cases worldwide.

Hydrogen can be made from water with light – but it's tricky

2023-05-20

One possible method is called photocatalysis: using light to induce and speed up the reaction.

An international team of researchers has been working on improving a chunk of the hydrogen photocatalysis reaction.

"Photocatalysis is an emerging alternative to electrocatalysis," says Professor Gunther Andersson, a researcher at Flinders University's College of Science and Engineering.

"It's not as mature a technology as electrocatalysis yet, but it's definitely an alternative."

Electrocatalysis is how most zero-emissions hydrogen is currently made at scale – using renewable electricity to split water (H2O) into hydrogen (H2) and oxygen (O2).

Photocatalysis creates the same reaction, but instead of electricity it harnesses sunlight directly.

Like many chemical processes, it uses catalysts – substances which make reactions easier – to do the job.

"A photocatalyst is basically absorbing the light and turning the light into something which then can be used for the reaction," explains Andersson.

"But there are a few other things needed to make it efficient. One is the so-called 'co-catalysts', which don't contribute to the absorption of light, but they help the water-splitting reaction happen efficiently."

Another problem is that, left to their own devices, any created hydrogen and oxygen gases will react together and turn back into water.

"The catalyst can work in two directions: you can split water to hydrogen and oxygen, but it likewise can do the opposite, and facilitate the reaction of hydrogen and oxygen to form water again. We call that the back reaction, and that's what you want to avoid," says Andersson.

One of Andersson's collaborators has shown that a layer of a substance called chromium oxide can efficiently prevent the back reaction from happening – but it's not perfect.

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"The whole work is now about the stability of the chromium oxide layer," says Andersson.

Andersson and colleagues have been looking into the properties of chromium-oxide layers over different catalysts and co-catalysts, while they're being annealed (basically heated). They've published their findings in ACS Applied Materials & Interfaces.

The researchers showed that the stability of the chromium depends on the catalyst or co-catalyst it's sitting on.

They also found that chromium oxide doesn't interfere with the overall water-splitting reaction.

"World-leading photocatalysts have chromium oxide overlayers, and this work reveals new insights into the nature of the coating that could lead to improvements in future materials," says co-author Professor Gregory Metha, a chemist at the University of Adelaide.

Researchers are working to come up with a suite of catalysts and co-catalysts that make photocatalytic hydrogen production competitive with existing methods.

"The holy grail of photocatalysis is getting to materials which absorb light in the visible part of the spectrum," says Andersson.

cosmosmagazine.com, 20 April 2023

https://cosmosmagazine.com

New molecule chops up RNA of "undruggable" common cancer-causing gene

2023-05-28

The MYC gene plays a key role in regulating cell proliferation, metabolism and controlled cell death, but it's not always helpful. In fact, it's been implicated in as many as 70% of all human cancers, covering a wide range of types of the disease, and overexpression is associated with worse outcomes for patients.

That makes it an attractive target for treatment, but unfortunately, it's not that simple. The associated MYC protein has a strange shape that makes it hard for drug molecules to latch onto, leading it to be considered mostly undruggable.

But a new study might be a step towards changing that. Researchers at The Wertheim UF Scripps Institute, Max Planck Institute, and the University of Münster have developed a way to bypass the tricky protein and shut down the gene by instead targeting its messenger RNA (mRNA). These molecules transcribe DNA to produce proteins, so interrupting that process can prevent the proteins being made rather than inactivating those already produced.

First, the team designed compounds made from imidazole that strongly bound to the mRNA of the MYC gene, as well as two other RNAs linked to cancer, JUN and microRNA-155. Binding alone didn't seem to help much, so the researchers added an extra structure to their molecules. This was designed to work like a fishing hook to catch enzymes that recycle RNA, and direct them to degrade the attached RNA. And sure enough, early results looked promising.

"With the degrader added, we started seeing these 'undruggable' cancer RNAs reduced by 35%, 40%, 50% or more," said Matthew Disney, lead author of the study. "This caused cancer cells to die and cleared tumors in mouse-based studies of breast cancer that spread to lungs."

Of course, it's still very early days for the technique, and the researchers say they still have a "marathon" ahead of them before it could reach human clinical trials. But it adds new hope for future treatments of many human cancers and other diseases.

"The compounds are a good starting point and show us where to go to build small molecules, RNA-targeting medicines that could eventually treat patients with diseases like aggressive cancers that currently have poor or no options," said Disney. "This new data also shows us that this approach could have many other disease applications."

A gene called MYC is implicated in the majority of cancers, but unfortunately, it's often considered "undruggable." In a new study scientists have developed a molecule that chops up the RNA of this gene, effectively clearing cancer in mice.

Other scientists have had some success treating this undruggable cancer gene by going after different targets, including downstream proteins or suppressing the MYC gene itself.

The new research was published in the journal Nature.

Source: Max Planck Institute

newatlas.com, 28 May 2023

https:// newatlas.com

Sunlight-powered catalyst transforms methane into valuable chemicals

2023-05-29

This innovative material, derived from tungsten trioxide (WO3 catalyst), features a dual active site comprising copper and tungsten atomic species that work in tandem to ensure an effective and selective conversion process. The conversion process can achieve nearly 100% selectivity under visible light, which avoids unwanted byproducts and increase efficiency, making it an eco-friendly alternative to current production methods. The findings have just been published in the journal Nature Communications.

Change the unchanged: Methane conversion

Methane, the principal component of natural gas, is a widely used carbon source for numerous chemicals. Nevertheless, it is also a potent greenhouse gas, with more than 70 times the global warming potential of carbon dioxide. The catalytic conversion of methane (converting methane into other chemicals), therefore, presents a tremendous opportunity for achieving net-zero energy and chemical supplies while simultaneously addressing environmental concerns.

However, methane is an extremely stable molecule, making it resistant to activation, particularly under mild or ambient conditions. Thus, achieving high activity and selectivity in methane conversion is a significant challenge, and the selective activation of the intermolecular carbon-hydrogen bond is often considered by many chemists as one of the most elusive "holy grails" in catalysis.

In a concerted effort with collaborators from the University College London, Professor Zhengxiao Guo from the Department of Chemistry, The University of Hong Kong (HKU), and Professor Junwang Tang, now at the Department of Chemical Engineering, Tsinghua University, have jointly developed a highly active and selective catalytic material that can efficiently convert methane, a potent greenhouse gas, into formaldehyde, an essential chemical in a waste-free manner.

Formaldehyde, on the other hand, is a high-volume commodity chemical with a market value of USD 8 billion, expanding at a compound annual growth rate (CAGR) of 5.7%. It is used in household, commercial, aviation, medical and automotive products and serves as a valuable precursor for melamine, urea-formaldehyde and phenolic resins, among others. Formaldehyde is also safely used in the manufacture of vaccines, anti-infective drugs and hard-gel capsules. Currently, it is produced through methanol oxidation-dehydrogenation using silver or metal-oxide catalysts at high reactor temperatures of more than 500°C–600°C, resulting in substantial carbon dioxide emissions and energy penalties.

Harnessing sunlight to convert methane

In their study, the team discovers a new way of turning methane gas into formaldehyde using sunlight. They found that a mixture of atomically dispersed copper and partially reduced tungsten species over tungsten oxide worked really well—the synergistic ensemble enabling exceptional photocatalytic methane conversion to formaldehyde under ambient visible light. The process exhibited nearly 100% selectivity and high conversion efficiency, significantly outperforming previously reported photocatalysts (with a turnover frequency, TOF = 8.5×106 μmol (HCHO)·g-1(cocatalyst)·h-1).

Through mechanistic analysis, they figured out that the copper helped to move electrons around and create reactive molecular species while the tungsten helped to activate the methane gas. Specifically, the copper acted as electron acceptors and promoted photo-induced electron transfer from the conduction band to dioxygen, generating reactive hydroperoxyl radicals (HOO·). Meanwhile, the adjacent tungsten atom that had a partial positive charge functioned as hole acceptors. The preferred adsorption and activation site of water produced hydroxyl radicals and effectively activated methane to methyl radicals. The synergy of the adjacent dual active sites greatly enhances the overall efficiency and selectivity of the conversion process.

This finding paves the way for further research and development of new photo-catalysts for a variety of chemical conversions, promoting more sustainable and efficient processes in the chemical industry.

"Solar conversion of methane is highly desirable for both low-carbon and high-value-added chemical syntheses. However, product selectivity and production efficiency are key to success. This requires an in-depth understanding of the conversion mechanism, careful design of the catalyst, and complementary techniques to confirm its performance—a

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good case of multidisciplinary tasks that require strong collaborative dedication. That's exactly what the team has managed to do—with much value-added outcome," said Professor Zhengxiao Guo, one of the corresponding authors of the paper.

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How a better understanding of mercury transformation can make ecosystems safer

2023-05-29

Mercury spread in the environment is a critical issue, due to the severe effects on human health and ecosystems. The main mercury exposure for humans comes from consuming fish with elevated mercury concentrations, especially in the form of methylmercury. Most of the methylmercury in the environment is formed by specific microorganisms by transforming mercury.

Mareike Gutensohn, at the Department of Chemistry at Umeå University, has explored how small sulfur-containing substances, called thiols, influence this transformation. Thiols can be found dissolved in oxygen-free waters or within the surface of cells, as part of proteins, and they play a critical role in forming methylmercury since they can attach to mercury and affect how easily it is transformed or absorbed by microorganisms.

Monitoring the environment is important

In her thesis, she has investigated systematically the combined effect of chemical and biological factors on the formation of methylmercury and the mechanistic behind it. The study unveiled that the formation of dissolved thiols, tied to cell metabolism, leads to enhanced production of methylmercury.

"The formation of both thiols and methylmercury heavily depends on the metabolic activity of microorganisms. Interestingly, the composition and concentration of the formed thiols significantly impact the potential for methylmercury formation. This underlines the importance of monitoring the formation of thiols within the environment," says Mareike Gutensohn, doctoral student at the Department of Chemistry.

The research also provided the first systematic characterization of the outer and inner cell membranes of the studied microorganism, with respect to thiols within the surface of the cells. For this, Mareike

A new study at Umeå University provides insight into how mercury transforms into its more toxic form, methylmercury, with the help of small sulfur-containing substances known as thiols.

Gutensohn used advanced spectroscopic techniques known as X-ray absorption spectroscopy, a powerful method to study cell-mercury interaction.

Complex relationship

The characterization unveiled variations in thiol concentration across the cell membrane, shedding light on the complex relationship between thiols and mercury transformation.

"While our understanding of thiols' role in methylmercury formation has significantly improved, there's still much to explore, particularly the role and implications of the differences in thiol concentration within the cell surface," says Mareike Gutensohn.

This study advances our understanding of the complex interplay of chemical and biological factors impacting mercury's transformation into methylmercury. This breakthrough in scientific understanding helps predict and control methylmercury formation, contributing to a safer and healthier ecosystem.

phys.org, 29 May 2023

https://phys.org

Why more foam makes for the best beer-drinking experience—and always has

2023-05-29

Too much froth and you're left with a smear of bubbles across your face and hanging from your nose as you desperately try to get at the beer beneath. But too little will cause problems in your stomach.

You see, if there's no foam the CO2 stays dissolved in the beer. If you then eat something, the foam erupts in your stomach rather than the glass, causing beer bloat. That's why tipping a glass to avoid a frothy head is a rookie error.

Hoping to solve this issue, a company in Japan has designed a beer can with two pulls, which control the level of foam produced by opening the can, resulting in the perfect amount of froth.

This is just the most recent development in beer technology. Humanity has been chasing the perfect pint since beer's inception, which evidence

What makes for the ultimate beer drinking experience? Some like theirs in a frosty glass, others with a wedge of lime. But when it comes to froth—or the head as it's commonly known—what's the best amount and how can it be achieved?

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suggests was roughly 13,000 years ago near Haifa, Israel—the oldest known record of human-made alcohol.

Under pressure

Beer consumption has evolved through the ages.

Those first producers and consumers of beer in Israel were the Natufian people, a group of hunter-gatherers in the eastern Mediterranean. Their beer would have been unfiltered, which made it look like thin porridge.

This led to the invention of beer straws around the fifth to the fourth millennium in Iran and Iraq, which featured a filter on the tip that held back the beer solids. These straws were similar in design to a modern bombilla (a yerba mate tea straw used for at least four centuries in South America).

The next significant leap in brewing was not the glass bottle, but another airtight closure: the barrel.

Advances in cooperage (the making of wooden casks and barrels) during the Middle Ages meant that the CO2 produced by yeast during fermentation remained in the solution within the container, rather than dissipating and giving it the porridge-like consistency of previous beers. This meant beer could be held and dispensed under pressure for the first time. This inexorably altered the appearance and flavor of beer, as it became effervescent and foamy when served fresh.

Foam was a vital component of proper beer because it showed its freshness.

A good head

The foamy head was at one time called a "collar"—a term that first appeared in print in John Steinbeck's 1945 novel Cannery Row. There seems to be no origin story attached to the moniker. And sadly, there seems less need to apply a name to beer foam since society has strayed from proper beer pouring techniques.

Traditionally, beer was allowed to foam up so much as it was being poured that a "foam scraper" (also known as a "foam flipper" or "head cutter") was needed to shave the excess off the glass rim. A large head was achieved by pouring the beer in an upright glass and encouraging excessive foaming. This technique dissipates the trapped CO2 and brings positive flavor elements to the forefront.

These days you'll notice that glasses are tipped while beer is poured. This is done to minimize foam but leads to a less pleasurable, gaseous experience instead of a creamy, toasty sip.

Next time you order a pint you should ask your bartender to pour the amber stuff into an upright glass. This is all to say, don't fear the foam, it's integral to your enjoyment.

phys.org, 29 May 2023

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New-look infrared lens shines a light on future technology and manufacturing

2023-05-29

Thermal and infrared imaging are used in many industries including defense, security and surveillance, medicine, electrical engineering, space exploration and autonomous vehicle operation—but the materials required are expensive and becoming more difficult to find.

Lower cost alternatives are needed so a multi-disciplinary team in chemistry and physics at Flinders University have developed a solution in an entirely new polymer material made from sulfur and cyclopentadiene. They say the high-performance polymers have the unique ability to transmit infrared light.

"The material combines high performance, low cost and efficient manufacturing," says Ph.D. candidate Sam Tonkin, first author in a new article in the Advanced Optical Materials journal.

"It has the potential to expand the use of thermal imaging to new industries which were previously limited by the high cost of germanium or chalcogenide lenses. This is a rapidly developing field which will see exciting advances in the next few years," he says.

Sulfur is produced in many millions of tons in petroleum refining. Billions of tons are available in geological deposits. It is plentiful and cheap.

Cyclopentadiene is also derived from low-cost materials produced in petroleum refining.

The lenses used for thermal imaging are currently made from germanium or chalcogenide glasses. Germanium is an element in short supply and it is very expensive. Some germanium lenses can costs thousands of dollars.

Researchers at Flinders University have discovered a new low-cost material that can be made into lenses for thermal imaging—pointing to new advanced manufacturing applications for this powerful technology.

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Chalcogenide glasses also have shortcomings. For instance, they are often made of toxic elements such as arsenic or selenium.

Co-author Dr. Le Nhan Pham, a Flinders University researcher in computational and physical chemistry, says reacting sulfur and cyclopentadiene together provides a black plastic with high transparency to infrared light.

"This is the light that is detected by thermal imaging cameras.

"This novel material was designed to have a wide array of potential applications from space engineering to military operation, and to civil and aerospace industries," he says.

The polymer can be molded into a variety of lenses, which can be used, for example, to magnify the image in a thermal camera. Because the polymer is black, it can also be used to conceal and protect thermal imaging equipment. The polymer can therefore be used as camouflage to hide a camera used for surveillance.

The infrared light passes through the polymer, so one can see through it using an infrared camera. This property is useful for defense operations and wildlife surveillance.

The polymer also has many other features:

- The material has the highest long-wave infrared light transparency ever reported for a plastic.
- The raw materials are low cost: for a 1 g lens the building blocks cost less than 1 cent.
- The material allows rapid molding into various shapes such as lenses. This is a more rapid process than current lens production which relies on slow milling methods.

The study also reported some key scientific advances, including a new reactor that was designed to enable the key reaction. A key challenge was to be able to use the building blocks in gaseous form. The use of gaseous monomers was previously thought not to be possible by other researchers in the area.

The study also includes quantum mechanical calculations to understand how and why the material is transparent to infrared light used in thermal

imaging. These insights will also be useful in the future to design new lenses with further improved properties.

phys.org, 29 May 2023

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Scientists use AI to find promising new antibiotic to fight evasive hospital superbug

2023-05-25

The process they used could also speed the discovery of other antibiotics to treat many other challenging bacteria.

Scientists at McMaster University and the Massachusetts Institute of Technology have used artificial intelligence to discover a new antibiotic that could be used to fight a deadly, drug-resistant pathogen that strikes vulnerable hospital patients.

The researchers were responding to the urgent need for new drugs to treat Acinetobacter baumannii, identified by the World Health Organization as one of the world's most dangerous antibiotic-resistant bacteria. Notoriously difficult to eradicate, A. baumannii can cause pneumonia, meningitis and infect wounds, all of which can lead to death.

A. baumanni is usually found in hospital settings, where it can survive on surfaces for long periods. The pathogen is able to pick up DNA from other species of bacteria in its environment, including antibiotic-resistance genes.

In the study, published today in the journal Nature Chemical Biology, researchers report they used an artificial intelligence algorithm to predict new structural classes of antibacterial molecules, and identified a new antibacterial compound, which they have named abaucin.

Discovering new antibiotics against A. baumannii through conventional screening has been challenging. Traditional methods are time-consuming, costly, and limited in scope.

Modern algorithmic approaches can access hundreds of millions, possibly billions, of molecules with antibacterial properties.

Lead author Jonathan Stokes, assistant professor in the Department of Biochemistry & Biomedical Science at McMaster University. Researchers identified a new antibacterial compound to treat the pathogen Acinetobacter baumannii. Credit: McMaster University

"This work validates the benefits of machine learning in the search for new antibiotics," says Jonathan Stokes, lead author on the paper and an assistant professor in McMaster's Department of Biomedicine &

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Biochemistry, who conducted the work with James J. Collins, a professor of medical engineering and science at MIT, and McMaster graduate students Gary Liu and Denise Catacutan.

"Using AI, we can rapidly explore vast regions of chemical space, significantly increasing the chances of discovering fundamentally new antibacterial molecules," says Stokes, who belongs to McMaster's Global Nexus School for Pandemic Prevention and Response.

"AI approaches to drug discovery are here to stay and will continue to be refined," says Collins, Life Sciences faculty lead at the MIT Abdul Latif Jameel Clinic for Machine Learning in Health. "We know algorithmic models work, now it's a matter of widely adopting these methods to discover new antibiotics more efficiently and less expensively."

Abaucin is especially promising, the researchers report, because it only targets A. baumannii, a crucial finding which means the pathogen is less likely to rapidly develop drug resistance, and which could lead to more precise and effective treatments.

Most antibiotics are broad spectrum in nature, meaning they kill all bacteria, disrupting the gut microbiome, which opens the door to a host of serious infections, including C. difficile.

"We know broad-spectrum antibiotics are suboptimal and that pathogens have the ability to evolve and adjust to every trick we throw at them," says Stokes. "AI methods afford us the opportunity to vastly increase the rate at which we discover new antibiotics, and we can do it at a reduced cost. This is an important avenue of exploration for new antibiotic drugs."

phys.org, 25 May 2023

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Study unlocks key information on major drug target for psychiatric and cognitive disorders, including schizophrenia

2023-05-30

An international study led by Monash University has, for the first time, harnessed cutting-edge technology to reveal new and unprecedented information of how a special class of drugs, known as "allosteric modulators" work at the M4 muscarinic receptor, a major target for notoriously difficult-to-treat psychiatric disorders associated with cognitive deficits, such as schizophrenia.

Muscarinic receptors are members of the superfamily of G protein-coupled receptors (GPCRs)—the largest drug target class encoded by the human genome. The M4 muscarinic receptor subtype, in particular, plays a vital role in regulating neurotransmitters, such as dopamine and glutamate, in key areas of the brain involved in psychosis and cognition, but, until

recently, was notoriously difficult to selectively target by conventional agonists or antagonists.

This challenge has begun to be addressed in recent years with the discovery of highly selective allosteric modulators for this receptor, but how such drugs achieve their selectivity and regulate M4 receptor activity in response to different activators has remained a major, elusive, knowledge gap, despite high clinical implications.

The new study, published in eLife, and led by a team of researchers from the Monash Institute of Pharmaceutical Sciences (MIPS), has now addressed this important gap in our molecular-level understanding of how allosteric modulators mediate their effects at the M4 muscarinic receptor.

In this study, the MIPS researchers (who are world-leaders in the discovery and development of next-generation neuromedicines, including allosteric modulators, for difficult-to-treat mental illnesses), rigorously quantified the pharmacological properties of two distinct 'positive' allosteric modulators, alone or in combination with two different agonists, at the human M4 muscarinic receptor.

The team also tapped into technological advancements in the fields of cryo-electron microscopy (cryo-EM) and molecular dynamics simulations to unlock first-of-its-kind evidence of key molecular mechanisms underlying allosteric pharmacology, advancing our understanding of the structural basis of allosteric modulation of the M4 muscarinic receptor and paving the way for the discovery and design of future allosteric drugs.

In particular, the researchers revealed a vital role for ligand–receptor–G protein complex stability, mediated by conformational dynamics between these sites, in the ultimate determination of affinity, efficacy, degree of allosteric modulation, and mechanisms underlying species variability of allosteric drugs, all of which have significant implications for preclinical-to-clinical discovery and translation of such agents.

Corresponding author, and MIPS Senior Research Fellow, Dr. David Thal, said that allosteric modulation of GPCRs is a major paradigm in drug discovery; however, despite decades of research, a molecular-level understanding of the general principles that govern the myriad pharmacological effects exerted by GPCR allosteric modulators has remained elusive.

"By determining the cryo-EM structures of the M4 muscarinic receptor and applying molecular dynamics simulations, the team has provided a holistic

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framework for further GPCR mechanistic studies and, in turn, opened up new approaches for GPCR drug discovery," said Dr. Thal.

Professor Arthur Christopoulos, FAA FAHMS, also a corresponding author on the study, Dean of the Faculty of Pharmacy and Pharmaceutical Sciences, and Director of Monash's Neuromedicines Discovery Centre, said the results have broader implications for the development of new allosteric medicines designed to reduce currently untreated symptoms associated with schizophrenia and cognitive disorders.

"The vast majority of patients with schizophrenia have impaired cognition, which is untreated by any existing antipsychotic drug, and its severity remains a major predictor of prognosis. However the development of new safe and effective treatments has remained stagnant for decades," said Professor Christopoulos.

"The research conducted in this study is a vital step toward progressing the next generation of medical therapies and innovations that could make a true impact when it comes to improving health and saving lives."

Dr. Celine Valant, also a corresponding author and Senior Research Fellow at MIPS, said the findings open up exciting new opportunities.

"The evidence presented in this study will enable future GPCR drug discovery research and potentially lead to the development of next generation medicines for the treatment of a range of psychiatric and cognitive disorders," said Dr. Valant.

phys.org, 30 May 2023

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Team develops novel algorithm for sharper protein films

2023-05-30

Sometimes, when using the navigation system while traveling by car, the device will locate you off the road for a short time. This is due to the inaccuracy of the GPS positioning, which can be as much as several meters. However, the algorithm in the sat nav will soon notice this and correct the trajectory displayed on the screen, i.e. put it back on the road.

A comparable principle for addressing unrealistic motion sequences has now been successfully applied by a team of researchers led by PSI physicist Cecilia Casadei. However, their objects of investigation are about a billion

Proteins are biological molecules that perform almost all biochemical tasks in all forms of life. In doing so, the tiny structures perform ultra-fast movements. In order to investigate these dynamic processes more precisely than before, researchers have developed a new algorithm that can be used to evaluate measurements at X-ray free-electron lasers such as the SwissFEL more efficiently. They have now presented it in the journal Structural Dynamics.

times smaller than a car: proteins. These building blocks of life fulfill crucial functions in all known organisms. In doing so, they often perform ultra-fast movements. Analyzing these movements precisely is crucial for our understanding of proteins which can help us produce new medical agents, among other things.

How to 'film' proteins

To further improve the understanding of protein movements, Casadei, together with other PSI researchers, a researcher at DESY in Hamburg and other colleagues at the University of Wisconsin in Milwaukee, U.S., has developed an algorithm that evaluates data obtained in experiments at an X-ray free-electron laser (XFEL). An XFEL is a large-scale research facility that delivers extremely intense and short flashes of laser-quality X-ray light. Here, a method called time-resolved serial femtosecond X-ray crystallography (TR-SFX) can be used to study the ultra-fast movements of proteins.

The measurements are very complex for several reasons: the proteins are much too small to be imaged directly, their movements are incredibly fast, and the intense pulse of X-ray light of an FEL completely destroys the proteins. On the experimental level, TR-SFX already solves all these problems: no individual molecule is measured, but rather a large number of identical protein molecules are induced to grow together in a regular arrangement to form protein crystals.

When the FEL X-ray light shines on these crystals, the information is captured in time before the crystals and their proteins are destroyed by the pulse of light. The raw data from the measurements are available as so-called diffraction images: light spots that are created by the regular arrangement of the proteins in the crystal and registered by a detector.

How to evaluate the measurement data

Where the experimental challenges have been overcome, the evaluation of the data is just beginning. "The measurement of each individual crystal provides only two percent of the data of a complete image." This incompleteness has physical and experimental reasons and can only be eliminated by combining the measurement data of many crystals in a meaningful way. Casadei's research focuses on exactly how to go about this.

The method established so far is called "binning and merging".

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"A lot has been achieved with this method in the last decade," says Casadei. With this method, the data are divided into time intervals and all data within one interval, a 'bin,' are averaged. However, a lot of detailed information is also lost in this averaging. "You could say that the individual images of the protein film are then all a bit washed out," Casadei continues. "That's why we have developed a method that allows us to get more out of the measurement data."

The new method devised by Casadei and her colleagues is called "low-pass spectral analysis", or LPSA for short. "Similar to electronics or audio technology, we apply a low-pass filter," Casadei explains. "However, in our case it comes in the form of advanced linear algebra. We apply these formulas to remove unwanted noise from the data without losing the relevant details."

In short and simple terms, the raw data, i.e. the diffraction images of the protein crystals, are tracked throughout the protein motion. This movement is assumed to be smooth, i.e. jerk-free. Similar to how the navigation system corrects itself when the car seemingly leaves the course of the road, the new algorithm by Casadei and her colleagues mitigates errors of the protein movement reconstruction.

HDR for protein films

Lay people may not notice an immense difference in the new protein films. But for the cineastes at X-ray free-electron lasers, the improvement is comparable to switching from a DVD film to HDR quality.

"Above all, the new algorithm now allows researchers here at SwissFEL at PSI to extract more information from their data," says Casadei. Conversely, this means the algorithm can help shorten long measurement times. Since beam time is always in high demand at large-scale research facilities, and in particular at SwissFEL, this is a most welcome prospect for protein researchers using this highly advanced facility.

phys.org, 30 May 2023

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Researchers develop method to probe supercooled water using electron diffraction

2023-05-30

Researchers at EPFL have found a way to study water in "no man's land," a subzero temperature range where water crystallizes rapidly. Historically, the inability to access "no man's land" has prevented scientists from unriddling the anomalous nature of water, but the breakthrough method can now change that.

Water is one of the most essential and widespread compounds on Earth. Covering over 70% of the planet's surface, it has shaped its composition

and geology, it regulates its climate and weather patterns, and is at the foundation of all life as we know it.

But water is also weird. It exhibits a number of anomalous properties, of which scientists have identified over seventy—so far. Several theories try to explain these anomalies, but verifying them experimentally is difficult. One of the reasons is that this would require studying water between 160 K and 232 K (-113 °C to -41 °C), a notorious temperature range known as "no man's land" where water crystallizes so fast that it has been impossible for scientists to study its properties.

But why would anyone want to cool water to such low temperatures? Because when water is cooled way below its freezing point it becomes 'supercooled' with unique and fascinating properties; for example, under certain conditions it can remain in liquid form but can freeze instantly when disturbed or exposed to certain substances. Supercooled water is obtained by taking liquid water and cooling it below the freezing point while using tricks to prevent it from crystallizing or at least slowing this process down. However, even with these tricks, crystallization in 'no man's land' is still too fast.

"An experiment to systematically probe the structure of water across so-called 'no man's land' has remained elusive for decades," says Professor Ulrich Lorenz at EPFL's School of Basic Sciences. Now, scientists led by Lorenz have found a way to do just that. The team developed a way to rapidly prepare deeply supercooled water at a well-defined temperature and probe it with electron diffraction before it can crystallize.

"We have still not fully understood why water is an anomalous liquid, despite this topic being hotly debated for over forty years," says Lorenz. "The answer appears to lie in 'no man's land." But because of fast crystallization, any measurement over the full temperature range has not been possible. We do this for the first time. This brings us closer to solving this long-standing mystery."

The scientists performed the experiments with a specialized time-resolved electron microscope they custom built in their lab. They prepared the supercooled water at a well-defined temperature and probed it directly before crystallization occurred. To do this, they cooled a layer of graphene to 101 K and deposited a thin film of amorphous ice. They then locally melted the film with a microsecond laser pulse to obtain water in 'no man's land," and captured a diffraction pattern with an intense, high-brightness electron pulse.

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The researchers found that as water is cooled from room temperature to cryogenic temperatures, its structure evolves smoothly. At temperatures just below 200 K (about -73 °C), the structure of water begins to look like that of amorphous ice—a form of ice where water molecules are in a disordered state—unlike the tidy crystalline ice we are usually familiar with.

"The fact that the structure evolves smoothly allows us to narrow down the range of possible explanations for the origin of water anomalies," says Lorenz. "Our findings and the method we have developed bring us closer to unriddling the mysteries of water. It is difficult to escape the fascination of this ubiquitous and seemingly simple liquid that still has not given up all of its secrets."

The research is published in the journal Nature Communications.

phys.org, date

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Scientists develop probe that could unlock the mysteries of a vital cellular messenger and lead to new drug discoveries

2023-05-30

The research paper—recently highlighted as Pick of the Week in the journal, Chemical Science—showcases the researchers' innovative probe that binds to inositol pyrophosphate or '5-PP-InsP5".

5-PP-InsP5 plays a fundamental role in various biological processes, including cell growth, programmed cell death, and enzyme regulation, and new roles are still emerging with it recently being found to be a key regulator of blood glucose levels.

Due to its diverse roles in cellular processes, 5-PP-InsP5 is an attractive target for developing therapeutic drugs.

However, biomedical and drug discovery research relies on 'small molecule probes' to detect specific target molecules and, until now, no 5-PP-InsP5-specific probes existed.

The Loughborough University and University of Oxford research team—which includes Dr. Stephen Butler, Dr. Felix Plasser, and Professor Barry Potter—combined their chemical synthetic and computational modeling

A study by Loughborough University and the University of Oxford has led to the development of a small molecule probe that could deepen our understanding of a crucial cellular messenger and lead to the development of new therapeutic drugs.

expertise to create a probe specific to 5-PP-InsP5 that emits a bright red light upon binding.

The intensity and duration of this light can be measured to quantify the levels of 5-PP-InsP5 during different biological processes, paving the way for a deeper understanding of its precise functions, mechanisms, and therapeutic potential.

Of the importance of the research, Dr. Stephen Butler commented, "A key motivation in our lab is to develop molecular tools with real-world applications, so we're excited about the potential of the probe reported here as a drug discovery tool, that could enable high-throughput screening of drug-like molecules that modulate biological processes involving the cellular messenger 5-PP-InsP5.

"Other inositol pyrophosphates exist and are still emerging in biology, so methods to detect, synthesize and exploit these could also be necessary and will be facilitated by the probe design features established in this project."

Professor Barry Potter, of the University of Oxford, added, "I have spent almost all of my independent scientific career in research on inositol phosphates and feel that the advent of these new pyrophosphate messengers, with their emerging biological functions, is truly exciting for the field and calls for innovation.

"Our highly collaborative new paper presents a very timely technique to measure such a messenger for the first time and should enable a wealth of further developments in the area."

The co-lead authors of the study are Megan Shipton and Fathima Jamion, a Ph.D. and final year undergraduate student from Oxford and Loughborough, respectively.

Megan and Fathima said of their achievement in a joint statement: "We are delighted to work as part of this collaborative team to take some vital steps in helping further uncover the biological roles of 5-PP-InsP5.

"It's especially rewarding to see our combined work published in a top chemistry journal and we look forward to seeing how it fuels future research in this area."

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The research paper, titled "Expedient synthesis and luminescence sensing of the inositol pyrophosphate cellular messenger 5-PP-InsP5," is Chemical Science.

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