Bulletin Board

Contents

(click on page numbers for links)

REGULATORY UPDATE

ASIA PACIFIC

List of evaluations in progress – updated June 2023	3
New allergen labelling requirements coming into effect soon	3

AMERICA

How California OSHA's Proposed Indoor Heat Illness Prevention Regulations May Affect Employers
Clean Power Plan 2.0: EPA's Latest Attack on America's Electric Reliability6
Wisconsin Senate's Proposed Bill to Combat PFAS Contamination
Maine Amends Notification Requirement in PFAS-Containing Products Law7

EUROPE

Commission and industry players commit to make the textile sector
greener, more digital and competitive9
England bans single-use plastic food contact items10

INTERNATIONAL

World Food Safety Day 202310
Biodegradable polyactic acid does not degrade in marine
environment, study finds11

REACH UPDATE

ECHA sees broad use of alternatives for chemical safety assessment13

JANET'S CORNER

Natural Scientists15

HAZARD ALERT

Sodium Bicarbonate16

GOSSIP

PFAS, PFAS everywhere: How pristine are laboratory materials?......21

CONTACT US

JUN. 16, 2023

subscribers@chemwatch. net tel +61 3 9572 4700 fax +61 3 9572 4777

1227 Glen Huntly Rd Glen Huntly Victoria 3163 Australia

* While Chemwatch has taken all efforts to ensure the accuracy of information in this publication, it is not intended to be comprehensive or to render advice. Websites rendered are subject to change.

letin Board

Contents

Novel combination of two reactions creates new molecule	22
New material transforms light, creating new possibilities for sensors	22
Researchers discover a new way to develop drugs without side effects	23
Can biorefineries eliminate fossil fuels and petrochemicals?	25
Atomic force microscopy probes mechanochemical kinetics	25
Mechanochemistry makes gold salts that are soluble in organic solvents	s26
Molecular fossils solve evolutionary mystery	26
Atomic force microscopy probes mechanochemical kinetics	27

CURIOSITIES

Photosynthesis starts with a single photon, study shows	28
Researchers report light-controlled transport of biomolecules	
across the cell membrane	30
Scientists develop novel biosensing-membrane for glucose	
detection and monitoring	31
New research provides a rapid and non-destructive method for	
identifying honey's botanical origin	32
Light and nickel found to simplify cross-coupling reactions	33
Wireless sensor enables real-time spoilage alerts on food	35
A conductive self-healing hydrogel to create flexible sensors	36
Buckle up: A new class of materials is here	37
Scientists create fluorogenic probe to detect enzyme linked to early	
stage of Alzheimer's	38
New strategy using curcumin provides smart fluorescence for anti-	
counterfeiting	40

TECHNICAL NOTES

(Note: Open your Web Browser and click on Heading to link to section)41	1
CHEMICAL EFFECTS41	1
ENVIRONMENTAL RESEARCH41	1
PHARMACEUTICAL/TOXICOLOGY41	1
OCCUPATIONAL	1

CHEMWATCH

letin Board

Regulatory Update

JUN. 16, 2023

ASIA PACIFIC

List of evaluations in progress – updated June 2023 2023-06-09

We've updated our Rolling Action Plan to include 31 newly initiated evaluations. There are now 34 evaluations in progress. For each evaluation, we have listed the subject, reason and time period for completion (an estimated evaluation completion date).

Published date: 9 June 2023

Read More

AICIS, 09-06-2023

https://www.industrialchemicals.gov.au/news-and-notices/listevaluations-progress-updated-june-2023

New allergen labelling requirements coming into effect soon

2023-06-08

Food businesses are busily preparing for new allergen labelling requirements coming into effect in early 2024.

The changes will help ensure mandatory food allergen declarations are clear and consistent. This is good news for anyone with a food allergy, as it will make it easier to find and read allergen information, and allow for safer food choices. Food manufacturers will also have a clearer understanding of how allergens have to be labelled on their products.

The transition period for businesses to comply with the new requirements ends on 25 February 2024. The new requirements include:

- an updated list of allergens that need to be declared
- the declaration of allergen information in a specific format and location on food labels

• the use of simple, plain English terms for allergen declarations. After 25 February 2024, a two-year stock-in-trade period will apply. Food packaged and labelled before 25 February 2024 that complied with previous allergen labelling requirements can continue to be sold during this two-year period.



Bulletin Board

Regulatory Update

More information about the allergen labelling changes is available on the FSANZ website.

Read More

Food Standards ANZ, 08-06-23

https://www.foodstandards.gov.au/media/pages/foodstandardsnews/ Default.aspx

AMERICA

How California OSHA's Proposed Indoor Heat Illness **Prevention Regulations May Affect Employers**

2023-06-09

California experienced the worst heat wave in its history during the summer of 2022. According to NASA.gov, on September 7, 2022, 61 million people were under heat advisory warnings, with the majority of these people residing in California and Arizona.

In preparation for extreme heat certain to hit different parts of the country in the summer of 2023, workplace safety regulators at both the federal and local levels continue to rethink heat illness prevention measures and develop regulations. California Occupational Safety and Health Administration (OSHA) is one of the agencies that has proposed regulations for indoor settings. Some of the key elements of these new regulations include:

- Relying more on heat index measurements and limits rather than plain temperature measurements
- Including both indoor and outdoor regulations and control requirements
- Accounting for both weather-related heat and process-generated radiant heat sources
- Adding allowances for what California OSHA terms "clothing that restricts heat removal"

Read More

JD Supra, 09-06-23

https://www.jdsupra.com/legalnews/how-california-osha-s-proposedindoor-8296673/

CHEMWATCH lletin Board

JUN. 16, 2023

Regulatory Update Clean Power Plan 2.0: EPA's Latest Attack on America's

Electric Reliability 2023-06-23

Chairman Johnson, Ranking Member Tonko, and Honorable Members of the Committee, my name is Jay Duffy, and I am the litigation director at Clean Air Task Force (CATF), a non-profit organization. I've been an attorney with CATF for ten years. CATF's mission is to push the technology and policy changes needed to achieve a zero-emissions, high-energy planet at an affordable cost. n1 In furtherance of that mission, CATF advocates for and defends strong Clean Air Act pollution standards for power plants. CATF's legal, policy, and technical experts have advocated for strong Clean Air Act section 111 greenhouse gas emission standards since 2008. n2 That is when, in light of the Supreme Court's determination that greenhouse gases are an air pollutant subject to the Clean Air Act, n3 the Bush Administration first requested comment on if, and how, to regulate the carbon pollution from power plants under section 111. n4

In the following fifteen years, there have been two attempts at regulating existing power plant sources' outsized impact on climate pollution. n5 Along the way, we all have learned many lessons. While EPA's latest proposal can, and should be strengthened, it represents a reasonable approach--in line with the power sector's trends and trajectory while also abiding by the plain text of the Clean Air Act and recent Supreme Court decisions--to meaningfully reduce emissions from new and existing coal and gas fired power plants.

Read More

Energy Central, 09-06-23

https://energycentral.com/news/clean-power-plan-20-epas-latest-attackamericas-electric-reliability-0

Wisconsin Senate's Proposed Bill to Combat PFAS **Contamination**

2023-06-09

On June 5, 2023, the Wisconsin Senate's Natural Resources Committee held a public hearing on proposed Senate Bill 312, which aims to distribute \$125 million in state funding to address pollution of per- and polyfluoroalkyl (PFAS). PFAS are a diverse group of manmade chemicals used in hundreds of products, and are alleged to have "possible links" with



Bulletin Board

Regulatory Update

"adverse health outcomes," including low birth weight, cancer, liver disease and reductions in vaccine effectiveness. The Bill comes on the heels of municipalities across Wisconsin struggling with PFAS contamination in groundwater. Currently affected areas include Green Bay, Marinette, Madison, Wausau and the town of Campbell on French Island.

Key provisions in the Bill include grants for local governments and public water utilities to test for PFAS and dispose of PFAS-containing biosolids, as well as upgrades to infrastructure and facilities. Proposed Senate Bill 312 also provides an opportunity for owners of private polluted wells to apply for grants. The Bill would also prohibit the Wisconsin Department of Natural Resources (DNR) from requiring owners of abandoned industrial property to test for PFAS unless the agency has information the property is contaminated. It would also prohibit DNR from preventing or delaying a development project based on PFAS contamination unless the pollution poses a risk to public health, the project could further degrade the environment, or the entity looking to complete the project caused the original contamination through its own negligence.

Senate Bill 312, in its current draft, also requires DNR to obtain permission from private landowners to test their waters for PFAS, and puts the onus on DNR to begin remedial actions at any contaminated site where the responsible party is unknown or unable to pay for remediation. Moreover, a public water utility provider would not need State regulators' permission to upgrade its facilities to address PFAS contamination if costs are less than \$2 million, or 50 percent of operating expenses from the year prior. Finally, proposed Senate Bill 312 requires the University of Wisconsin and DNR to collaborate on PFAS treatment studies.

Read More

JDSupra, 09-06-23

https://www.jdsupra.com/legalnews/wisconsin-senate-s-proposed-billto-3435836/

Maine Amends Notification Requirement in PFAS-**Containing Products Law**

2023-06-09

What is happening? Maine has enacted an amendment to the state's statute regulating the use of perfluoroalkyl and polyfluoroalkyl substances (PFAS) in products. Under the law as originally passed, manufacturers of products containing intentionally added PFAS

CHEMWATCH

Bulletin Board

Regulatory Update

JUN. 16, 2023

were required to provide certain detailed information to the Maine Department of Environmental Protection (DEP) beginning January 1, 2023. The amendment extends this statutory deadline to January 1, 2025, and makes certain changes to the required substance of notifications. The amendment applies retroactively to January 1, 2023. The amendment does not alter the law's broad definition of PFAS, nor does the amendment alter the state's ban on non-exempt products containing intentionally added PFAS as of January 1, 2030. What is the background? Maine's original PFAS-containing products law was adopted in July 2021. Since then, Maine DEP has been developing, but has not yet finalized, regulations to implement the law. Maine DEP has acknowledged the difficulty in implementing the law's notification requirements. Thousands of companies have requested and received extensions to notification requirements beyond the statutory deadline.

Summary of Key Provisions

Reporting Deadline Extension. The statutory deadline for manufacturers to notify Maine DEP of their products for sale in the state that contain intentionally added PFAS has been extended by two years from January 1, 2023 to January 1, 2025.

Additional Requirement to Report Estimate of Total Units Sold. The amendment adds a requirement to report to Maine DEP an estimate of the total number of units of in-scope products sold annually in Maine or nationally.

New Methods of Reporting PFAS Amounts in Products Permitted. Under the original law, the amount of each PFAS in products was to be identified by its chemical abstracts service (CAS) Number and reported as an exact quantity or as falling within a range approved by Maine DEP. The amendment now allows PFAS to be identified through a Maine DEPapproved description. The amendment also authorizes reporting the amount of total organic fluorine if the amount of each PFAS compound in a product is unknown. Additionally, PFAS reporting can now be based on supplier-provided information rather than through testing. Exemption for Small Manufacturers. The amendment exempts from the statute's notification requirement a manufacturer that employs 25 or fewer people.

Read More

The National Law Review, 09-06-23

https://www.natlawreview.com/article/maine-amends-notificationrequirement-pfas-containing-products-law

Bulletin Board

Regulatory Update

JUN. 16, 2023

EUROPE

Commission and industry players commit to make the textile sector greener, more digital and competitive

2023-06-06

Today (6 June 2023), the European Commission published the transition pathway for the textiles ecosystem, which has been co-created by the Commission and relevant actors in the sector. The pathway defines specific actions to make this industry greener and more digital, and to ensure its long-term sustainability, resilience and competitiveness.

Through eight building blocks, the transition pathway outlines around 50 actions, including the promotion of circular and sustainable practices, services and business models and the support for SMEs to innovate, accelerate the twin transition, and to grow internationally.

It also includes actions on up-and reskilling, i.e., promoting access to lifelong learning and training opportunities for skilled workers. The report highlights the need to strengthen market surveillance for the textiles ecosystem and to make use of trade policies to promote exports and enforce environmental and social standards.

The Commission is now inviting all interested parties to contribute to the implementation of the transition pathway by putting forward their proposed commitments to support it.

The Commission proposed to develop transition pathways in different ecosystems in its May 2021 Industrial Strategy UpdateEN, as part of efforts to accelerate the green and digital transformation of the European industry. So far, transition pathwaysEN have been published in the fields of TourismEN, Proximity and Social EconomyEN, ChemicalsEN and ConstructionEN.

Read More

European Commission, 06-08-23

https://single-market-economy.ec.europa.eu/news/commission-andindustry-players-commit-make-textile-sector-greener-more-digital-andcompetitive-2023-06-06_en

Regulatory Update

CHEMWATCH

England bans single-use plastic food contact items 2023-06-08

On May 23, 2023, the UK's Department for Environment, Food & Rural Affairs (Defra) published its guidance on England's single-use plastics ban, concerning plates, bowls, trays, containers, cutlery, and balloon sticks. The guidance says that from October 1, 2023, businesses must no longer supply, sell, or offer these single-use plastic items in England.

Single use is defined as items that are meant to be used only once for their original purpose and include biodegradable, compostable, and recycled items. The document also includes exemptions from the ban such as supplying the items to another business, or items that are already acting as packaging: e.g., pre-filled salad bowl or ready meal packaged in a tray, a plate filled at the counter of a takeaway, a tray used to deliver food.

The ban also includes the supply of polystyrene food and drink containers. Exemptions here are if the product needs further preparation before being consumed, e.g., adding water, microwaving, or toasting.

The United Kingdom was part of the European Union during much of the development of the EU's single use plastics directive (FPF reported). England is the last of the four nations that make up the United Kingdom to incorporate single-use plastic bans into national law.

Read More

FPF, 08-06-23

https://www.foodpackagingforum.org/news/england-bans-single-useplastic-food-contact-items

INTERNATIONAL

World Food Safety Day 2023

2023-06-08

Today (7 June) is World Food Safety Day (WFSD), held annually to raise awareness of the many ways to prevent, detect and manage foodborne risks.

This year's theme — Food standards save lives — aims to draw attention to the role standards play in ensuring the food we eat is safe. Equally, it acknowledges the people who contribute to keeping our food supply safe by developing, maintaining and using food safety standards and practices.



Bulletin Board

Regulatory Update

FSANZ is proud of our work to develop and maintain the standards that help ensure food in Australia and New Zealand remains safe.

Among their many functions, food standards provide guidance on safe and hygienic food handling practices, define the maximum levels of additives, contaminants and residues permissible in food, and guide labelling requirements including nutrition and allergen information.

The critical work of standards setters here and internationally supports all levels of food production, from providing businesses with clear guidance on producing safe food through to ensuring people can consume food with confidence.

WFSD is an initiative of the United Nations and the World Health Organization (WHO). For more information on WFSD, see the WHO website.

Read More

Food Standards ANZ, 08-06-23

https://www.foodstandards.gov.au/media/pages/foodstandardsnews/ Default.aspx

Biodegradable polyactic acid does not degrade in marine environment, study finds

2023-05-24

A study published on May 24, 2023, in the Journal PLOS ONE examined the degradability of biodegradable plastics in a real marine environment. The authors used polylactic acid (PLA) as a biodegradable material. The study focused on PLA in textiles, however, it is the same chemical composition that is used for plastic food contact articles, such as single-use cutlery. For materials to be declared as biodegradable, certain requirements must be met. Yet, the way these requirements are tested oftentimes does not represent actual ecological environments - such as the ocean, where a lot of plastic items will end up. The environment that the materials are tested for resembles more industrial composting settings (FPF reported).

To test environmental degradation, the team led by scientists from the Scripps Institution of Oceanography at UC San Diego submerged pieces of bio-based PLA, as well as oil-based polypropylene (PP) and polyethylene terephthalate (PET) at the sea surface and at 10 m depth for a total of 428 days in a metal cage contraption. The results showed that the purportedly biodegradable PLA, together with the PP and PET, did not show any signs

CHEMWATCH lletin Board

Regulatory Update

of degradation after the testing period. Inspection with Raman spectra also did not show any chemical changes in the materials. In contrast, natural and regenerated cellulose-based fibers that were tested in the same way degraded completely within approximately 35 days.

Finally, the authors conclude that "referring to compostable plastics as biodegradable plastics is misleading as it may convey the perception of a material that degrades in the environment." Moreover, the scientists emphasize that the existence of degradable materials should not act as a rationale to continue a destructive and throw-away lifestyle.

For more information about plastics, the difference between bio-based and biodegradable, and the environmental and health impacts of these materials, the Food Packaging Forum has published short fact sheets with concise and scientific information on plastics, bioplastics, and more. Both factsheets are available in English, French, and Spanish.

Read More

JUN. 16, 2023

FPF,08-06-23

https://www.foodpackagingforum.org/news/biodegradable-polyacticacid-does-not-degrade-in-marine-environment-study-finds



Bulletin Board

REACH Update

JUN. 16, 2023

ECHA sees broad use of alternatives for chemical safety assessment

2023-05-30

The report shows that adaptations continue to be used more than experimental studies, with read-across being the most frequent option. In vitro non-animal test methods have seen a significant uptake in recent years.

Helsinki, 30 May 2023 – The European Chemicals Agency (ECHA) has published its fifth report on the use of alternatives to testing on animals for the REACH Regulation. The report finds that progress is being made in the increased use of alternatives to gather data on the properties of substances, in place of animal testing.

Similarly, to previous reports, the most common adaptation is read-across, where information from similar substances is used. This is followed by justifications for omitting data (data waiving), combining information from different sources (weight of evidence) and predicting properties from structurally similar substances using computer models (QSAR).

In recent years, there has been a notable increase in the use of in vitro test methods, which involve studies with cells, tissues, or organs. These are used specially to obtain data for skin corrosion/irritation, serious eye damage/eye irritation and skin sensitisation.

Around 50% of the studies conducted between 1990 and 2022 for skin and eye irritation have been performed in vitro. For new studies conducted in 2019-2022, this percentage rises to approximately 90%.

Today's report shows that alternatives to animal testing are widely used when assessing the safety of chemical substances and further progress is being made recently. We are committed to continue promoting the use of alternatives by contributing to the scientific debate and regulatory work to replace animal testing in the long term.

We are cooperating with the European Commission, and other partners, to support the development of policies that accelerate the pace for transition towards full replacement of animal testing.

The report sheds light on opportunities and challenges associated with moving away from animal testing in the regulatory assessment of chemicals. Additionally, it presents ECHA's initiatives to promote non-animal testing and to increase the acceptance and uptake of new approach methodologies.

REACH Update

CHEMWATCH

The Agency also engages in international collaborations such as Accelerating the Pace of Chemical Risk Assessment (APCRA), the European Partnership for the Assessment of Risks from Chemicals (PARC), the European Partnership for Alternative Approaches to Animal Testing (EPAA) and cooperates with the Organisation for Economic Co-operation and Development (OECD).

By facilitating easy access to toxicity data, ECHA supports research and development within the wider regulatory and scientific community.

To further explore new approach methodologies and work towards an animal testing-free regulatory system for industrial chemicals, ECHA will host a workshop on 31 May-1 June. The event can be followed online.

Read More

ECHA, 30-05-23

https://echa.europa.eu/-/echa-sees-broad-use-of-alternativesfor-chemical-safety-assessment#msdynttrid=ZjQKJjgZIPHvWo6-2pAZqK0JvtcjBkWhSrv8ctlkrnc



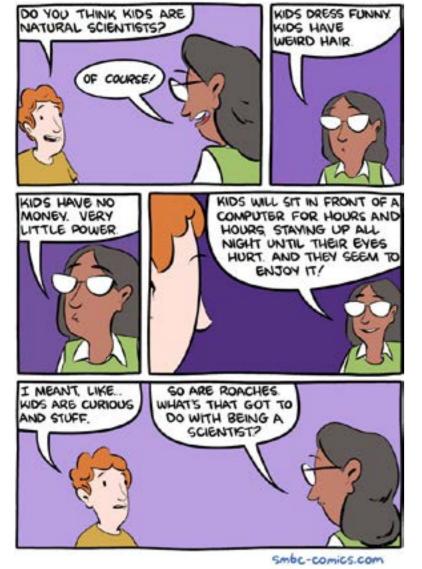


Bulletin Board

Janet's Corner

Natural Scientists

2023-06-16



https://www.smbc-comics.com/comic/natural-scientists

IUN. 16, 2023

Hazard Alert

CHEMWATCH

Sodium Bicarbonate

2023-06-16

USES [2,3]

Sodium bicarbonate is used across a range of applications in various industries. It is an alkaline solution, meaning it neutralises acids. In this capacity it is used as an antacid—for conditions such as heartburn and indigestion. It can also be used to help contrast-induced nephropathy, stomach ulcers, dental plaque, and tooth discolouration. Besides its use as an antacid, bicarbonate of soda is used in baking as a leavening agent.

ROUTES OF EXPOSURE [5]

Routes of Exposure

Sodium bicarbonate can be taken intravenously and orally.

HEALTH EFFECTS [4]

Sodium bicarbonate poisoning affects a range of systems, including the integumentary and respiratory systems.

Acute Health Effects [6]

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

If a high concentration of chemical dust is inhaled, it can result in coughing, sneezing, or a sore throat. If large amounts of the chemical compound are ingested, it can cause gastrointestinal problems or abdominal pain. Eye contact with the chemical can result in mild irritation, including temporary redness and temporary impairment of vision.

Chronic Health Effects [6]

Chronic exposure to sodium bicarbonate is toxic to multiple body systems. Long term skin exposure to the chemical may cause dermatitis, characterised by skin redness and swelling, which may cause blistering and scaling and thickening of the epidermis. Although this chemical is not thought to cause other long-term effects, exposure should be minimised as a matter of course.



IUN. 16, 2023

Sodium bicarbonate, aka baking soda or bicarbonate of soda, is a soluble odourless white crystalline powder. It is a salt that breaks down to form bicarbonate and sodium in water. [1,2,4]

letin Board

Hazard Alert

UN. 16, 2023

SAFETY

First Aid Measures [6]

Ingestion: If swallowed, immediately give the victim water to drink. First aid is usually not required; if in doubt, contact the poisons hotline.

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 soap and water. Contact a doctor in the event of continued irritation.

Eye contact: Flush eyes (including under the eyelids), with water for at least 15 minutes. Removal of contact lenses should only be done by skilled personnel. Contact a medical professional immediately.

Inhalation: If the person inhales fumes, combustion products or aerosols, remove them from the contaminated site. Other measures are usually unnecessary. If in doubt, contact the poisons information centre.

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

Personal Protection [5]

Engineering controls: Emergency eyewash fountains and guick-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 chemical dust in the air.

Personal protection: Safety glasses, protective and dustproof clothing, gloves, a P.V.C apron and an appropriate mask or dusk respirator. Wear impervious shoes. Other protection could include barrier cream and skin cleansing cream. For specifications regarding other PPE, follow the guidelines set in your jurisdiction.

REGULATION

United States

The Time Weighted Average (TWA) for sodium bicarbonate has been set at 10mg/m3.

Hazard Alert

CHEMWATCH

Australia [7]

No TWA has been set specifically for this chemical. Instead, there is a blanket limit of 10mg/m3 for dusts when no other limits have been specified.

REFERENCES

- 1. https://pubchem.ncbi.nlm.nih.gov/compound/Sodium-bicarbonate
- 2. https://www.webmd.com/vitamins/ai/ingredientmono-1470/sodiumbicarbonate
- 3. https://www.drugs.com/mtm/sodium-bicarbonate.html
- 4. https://www.msdsonline.com/2015/02/16/safety-with-sodiumbicarbonate/
- 5. https://en.wikipedia.org/wiki/Sodium bicarbonate
- 6. Jr.chemwatch.net
- 7. https://www.chemsupply.com.au/documents/SL0011CH6E.pdf
- 8. https://www.salchem.com/MSDS/S/Sodium_Bicarbonate.pdf





Bulletin Board

Gossip

JUN. 16, 2023

Researchers develop universal MHC molecules that can be produced rapidly at scale

2023-06-13

When foreign peptides are identified, they trigger a cascade that allows cytotoxic T cells to eliminate intruders. This process has been exploited in the development of both vaccines and immunotherapy, wherein researchers identify fragments of peptides unique to viruses or cancer and then screen for T cells that recognize those targets and initiate an immune response.

However, the current process of using MHC-I molecules as probes in vaccine and immunotherapy development is laborious. MHC-I molecules are extremely unstable, and making just one of these molecules can take a week, making it prohibitive to scan large libraries of peptides in an efficient manner.

Now, researchers from Children's Hospital of Philadelphia (CHOP) have potentially solved this problem by engineering stable, universal MHC-I molecules that can be produced rapidly at scale, allowing researchers not only to develop vaccines and immunotherapies more quickly but also to identify molecules that can work broadly across the population. The findings are published in the Proceedings of the National Academy of Sciences.

"The findings in this paper have the potential to revolutionize this field, both in the way we manufacture these molecules and the rate at which we can screen for effective and universal immunotherapies," said senior author Nikolaos G. Sgourakis, Ph.D., Associate Professor in the Center for Computational and Genomic Medicine at Children's Hospital of Philadelphia. "We are no longer limited by the instability of these molecules and the long timeframe it used to take to manufacture them. These stabilized MHC-I molecules could speed up the screening process and the subsequent development of effective therapies."

Led by Sgourakis Lab members Yi Sun, Michael C. Young, and Claire H. Woodward, the researchers stabilized MHC-I molecules by focusing on their 3D structure. Classical MHC-I molecules are comprised of three major parts: a peptide antigen consisting of 8 to 15 amino acids; a light chain that is the same for all MHC-I molecules; and a highly polymorphic heavy chain.

Class I major histocompatibility complex (MHC-I) proteins play an essential role in the immune system of all jawed vertebrates. The MHC-I displays peptide fragments of proteins from within the cell on the cell surface, "presenting" them to the immune system, which is constantly scanning the body for foreign or toxic antigens.

Gossip

CHEMWATCH

In humans, the MHC-I is called human leukocyte antigen, or HLA, which has expanded because of constant evolutionary adaptation in the human population to include more than 35,000 variants, with a variety of different residues located on groove where peptides can bind. Because HLA is so polymorphic, different HLA types display different peptide repertoires, bind different molecular chaperones, and display different T cell receptors (TCRs), which ultimately define immune responses and disease susceptibility. Thus, finding universal targets and immunotherapies that work across the human population has been challenging.

To stabilize MHC-I and make it useful for universal peptide loading and screening, the researchers focused on the light chain of the molecule, since it is conserved across HLA types. The light chain performs an important role in stabilizing MHC-I molecules. As soon as the light chain falls off, it triggers the MHC-I molecule to disassemble, at which point it is essentially sent for recycling for future peptide loading, serving as a sort of "on/off" switch for the MHC-I molecule. To exploit this fundamental engineering, the researchers tethered the heavy chain to the light chain, stabilizing the MHC-I in a conformation that is "open" and receptive to peptides.

The researchers confirmed the stability of these engineered MHC-I molecules through biophysical characterization, using nuclear magnetic resonance (NMR), showing that their open MHC-I molecules have enhanced stability when loaded with peptides, even those of low to moderate affinity. The researchers also demonstrated that their engineered MHC-I molecules promote peptide exchange across multiple HLA allotypes, covering representatives from five HLA-A, six HLA-B supertypes, and HLA-Ib molecules, which have many different forms.

A key component of using this system to enable a high-throughput peptide exchange platform was the design of customized "placeholder" peptides containing unnatural amino acid modifications, which was done in close collaboration with the lab of chemical biologist George Burslem, Ph.D., at the University of Pennsylvania.

"The open MHC-I platform leverages minimal protein modifications to enhance ligand exchange reactions across all known HLA allotypes, as well as oligomorphic MR1 molecules which present aberrant metabolites that are associated with many tumors," Dr. Sgourakis said. "These new molecules could be a versatile tool for screening antigenic epitopes,

letin Board

Bulletin Board

Gossip

enabling the detection of low-frequency receptors and engineered antibodies for the development of targeted therapies."

Phys Org, 13 June 2023

https://phys.org

PFAS, PFAS everywhere: How pristine are laboratory materials?

2023-06-13

Such toxicology studies often employee several types of "blanks" for quality control. Blanks are experiments where the test animals are not given any dose of the chemical being studied (sort of like a placebo in human drug testing). Also, researchers often examine the amount of the substance under study in the blanks to also include it in the evaluation of the dose versus effect relationship.

For example, if the study is in water, they may get water from a pristine site to use in the test and not add any chemical dose to it, but they would still analyze the water in order to detect any trace amounts of the study substance. Researchers would also analyze feed for the same reason.

One research group sought to examine how the presence of PFAS in test animal feed, test materials, and the animal subjects themselves may thwart the toxicology studies of the effect of PFAS and could lead to inaccurate results.

Matt Simcik and co-authors sampled minnows raised in aquaculture facilities (used for toxicity testing), as well as different types of fish food: flakes, freeze-dried brine shrimp, freeze-dried blood worms and frozen brine shrimp, for PFAS. Both fish and fish feed were found to be contain PFAS at varying levels. The study documents the differences between food type, brand, and aquaculture practices, but ultimately recommends that any all feed and organisms should be tested for PFAS contamination prior to conducting basic or translational experiments.

The research is published in Environmental Toxicology and Chemistry.

Phys Org, 13 June 2023

https://phys.org

How do you study the effects of exposure to per- and polyfluoroalkyl substances (PFAS), when it is in everything? To study the effect of a chemical, toxicologists typically expose animals to various doses of the chemical over a period of time so that they could then study the dose versus effect relationship.

CHEMWATCH

Bulletin Board

JUN. 16, 2023

Novel combination of two reactions creates new molecule

2023-06-13

Gossip

"This research was based on a very simple idea of combining two types of reactions," stated Professor Sakamaki. "However, it was not clear if these reactions could coexist because they are so different in nature. Our results are expected to contribute to the development of new synthetic components for functional materials, such as sensing materials and porous materials."

The study findings were published in Angewandte Chemie International Edition.

Phys Org, 13 June 2023

https://phys.org

New material transforms light, creating new possibilities for sensors

2023-06-12

"This process gives us a whole new way of designing materials," said Sean Roberts, an associate professor of chemistry at UT Austin. "It allows us to take two extremely different substances, silicon and organic molecules, and bond them strongly enough to create not just a mixture, but an entirely new hybrid material with properties that are completely distinct from each of the two components."

Composites are composed of two or more components that adopt unique properties when combined. For example, composites of carbon fibers and resins find use as lightweight materials for airplane wings, racing cars and many sporting products. In the paper co-authored by Roberts, the inorganic and organic components are combined to show unique interaction with light.

Among those properties are the ability to turn long-wavelength photons—the type found in red light, which tends to travel well though tissue, fog and liquids-into short-wavelength blue or ultraviolet photons, which are the type that usually make sensors work or produce a wide range of chemical reactions. This means the material could prove useful in new technologies as diverse as bioimaging, light-based 3D printing and light sensors that can be used to help self-driving cars travel through fog.

JUN. 16, 2023

A research group led by Professor Hideki **Fujiwara and Associ**ate Professor Daisuke Sakamaki from the **Graduate School of** Science at Osaka Metropolitan University succeeded, for the first time, in synthesizing a new molecule using a novel combination of dynamic covalent chemistry, in which organic radicals couple and dissociate reversibly, and coordination chemistry, which binds radicals to metal ligands. The study shows that the two types of reactions work without inhibiting each other.

Bulletin Board

Gossip

"This concept may be able to create systems that can see in near infrared," Roberts said. "That can be useful for autonomous vehicles, sensors and night vision systems."

Taking low energy light and making it higher energy also can potentially help to boost the efficiency of solar cells by allowing them to capture near-infrared light that would normally pass through them. When the technology is optimized, capturing low energy light could reduce the size of solar panels by 30%.

Members of the research team, which includes scientists from the University of California Riverside, University of Colorado Boulder and University of Utah, have been working on light conversion of this type for several years. In a previous paper, they described successfully connecting anthracene, an organic molecule that can emit blue light, with silicon, a material used in solar panels and in many semiconductors.

Seeking to amplify the interaction between these materials, the team developed a new method for forging electrically conductive bridges between anthracene and silicon nanocrystals. The resulting strong chemical bond increases the speed with which the two molecules can exchange energy, almost doubling the efficiency in converting lower energy light to higher energy light, compared with the team's previous breakthrough.

Kefu Wang and Ming Lee Tang of University of Utah, R. Peyton Cline and Joel D. Eaves of University of Colorado Boulder, Joseph Schwan and Lorenzo Mangolini of University of California Riverside and Jacob M. Strain of UT Austin also contributed extensively to the research.

Phys Org, 12 June 2023

https://phys.org

Researchers discover a new way to develop drugs without side effects

2023-06-08

If the cell membrane is like an Oreo cookie sandwich, GPCR is like a snake with seven segments traversing in and out of the cookie sandwich surface. The extracellular loops are the inbox for messages. When a message molecule binds to the extracellular side of the receptor, it triggers a shape change activating G proteins and the ß-arrestin protein attached to the intracellular side of the receptor. Like a molecular relay, the information

Have you ever wondered how drugs reach their targets and achieve their function within our bodies? If a drug molecule or a ligand is a message, an inbox is typically a receptor in the cell membrane. **One such receptor** involved in relaying molecular signals is a G protein-coupled receptor (GPCR). About one-third of existing drugs work by controlling the activation of this protein. **Japanese researchers** now reveal a new way of activating **GPCR by triggering** shape changes in the intracellular region of the receptor. This new process can help researchers design drugs with fewer or no side effects.

JUN. 16, 2023

CHEMWATCH

Illetin Board

Gossip

passes downstream and affects various bodily processes. That is how we see, smell, and taste, which are sensations of light, smell, and taste messages.

Adverse side effects ensue if drugs acting on GPCRs activate multiple signaling pathways rather than a specific target pathway. That is why drug development focuses on activating specific molecular signal pathways within cells. Activating the GPCR from inside the cell rather than outside the cell could be one way to achieve specificity. But until now, there was no evidence of direct activation of only the intracellular side of GPCRs without the initiations from the extracellular side.

A team of researchers headed by Osamu Nureki, a professor at the University of Tokyo, and his lab, discovered a new receptor activation mode of a bone metabolism-related GPCR called human parathyroid hormone type 1 receptor (PTH1R) without signal transduction from the extracellular side.

"Understanding the molecular mechanism will enable us to design optimal drugs," says Kazuhiro Kobayashi, a doctoral student and an author of the study. Such a drug offers "a promising treatment for osteoporosis."

Kobayashi has been conducting research on bone formation in animal models since he was an undergrad. "Treatments for osteoporosis that target PTH1R require strict dosage, have administrative restrictions, and there aren't yet any better alternatives," he says. That motivated their team to look for better drug design strategies targeting the parathyroid hormone receptor.

To understand function through structure, they used cryo-electron microscopy and revealed the 3D structure of the PTH1R and G protein bound to a message molecule. The team synthesized a non-peptide message molecule called PCO371 which binds to the intracellular region of the receptor and interacts directly with G protein subunits. In other words, PCO371 activates the receptor after entering the cell.

The PCO371-bound PTH1R structure can directly and stably modulate the intracellular side of PTH1R. And because PCO371 activates only G protein and not ß-arrestin it does not cause side effects. This specificity of its binding and receptor activation mode makes it a suitable candidate for potential small-molecule-based drugs for class B1 GPCRs, like PTH1R, which currently lack oral administrative drug ligands. Such drugs would have reduced adverse effects and burdens on patients as they act on specific molecular pathways.



Bulletin Board

Gossip

The findings from this study will help "develop new drugs for disorders such as obesity, pain, osteoporosis, and neurological disorders."

The study appears in the journal Nature.

Phys Org, 8 June 2023

https://phys.org

Can biorefineries eliminate fossil fuels and petrochemicals?

2023-06-12

Biorefineries are facilities that convert natural materials to fuels or chemicals. SGP Bioenergy's one will repurpose existing bunker fuel oil terminals together with new facilities at opposite ends of the Panama Canal, in Colon and Balboa, eventually producing 180,000 barrels (29 million litres) of biofuel per day. It will buy crops grown by farmers under contract, requiring 1.5 million acres (0.6 million hectares) of land, according to estimates (for reference, there are about 23 million acres of farmland in the UK).

Others see the purpose of biorefineries differently. Decarbonising the chemical sector using carbon-neutral biomass feedstocks that sequester carbon dioxide as they grow during photosynthesis could be a realistic target. In this scenario, biorefineries primarily co-produce energy for their own use, or supply biomass-based energy for poor marginalised communities. There is always competition for how to use land and care is urged in growing plants specifically to produce fuel or energy.

Chemistry World, 12 June 2023

https://chemistryworld

Atomic force microscopy probes mechanochemical kinetics

2023-06-13

Experiments probing how force accelerates chemical reactions have provided new insights into mechanochemical kinetics. The findings by USbased scientists could inform the development of chemical manufacturing methods that are more sustainable and less wasteful than current approaches.

Plans to develop the world's largest vegetable oil refinery reveal diverging views on the sustainability, profitability and scale of plantbased supply chains, **finds Andy Extance**

JUN. 16, 2023

Gossip

In mechanically activated organic chemistry, force drives the making and breaking of covalent bonds. This helps to minimise the waste and energy cost associated with organic synthesis because the reactions are run neat or with minimal solvent, and energy is provided through mechanical, rather than thermal, means.

Chemistry World, 13 June 2023

CHEMWATCH

https://chemistryworld

Mechanochemistry makes gold salts that are soluble in organic solvents

2023-06-07

A new one-pot mechanochemistry method for processing elemental gold can provide organosoluble gold salts in under one hour. By combining potassium peroxymonosulfate, a common pool cleaner, tetraalkylammonium halide salts and metallic gold in a solvent-free ball mill reaction, the technique avoids traditional harsh and toxic reagents used for gold oxidation.

Chemistry World, 7 June 2023

https://chemistryworld

Molecular fossils solve evolutionary mystery 2023-06-13

Fossilised 'protosteroid' molecules discovered in 1.6-billion-year-old rocks could be signs of a hidden world of ancient organisms belonging to the earliest forms of complex life. The finding suggests that short-lived precursors in modern steroid biosynthesis were once functional end products in their own right, solving a decades-old mystery surrounding the early evolution of eukaryotes.

Primordial precursors of modern steroid compounds were first posited by biochemist Konrad Bloch who helped decipher the biosynthetic pathway of cholesterol, co-winning the Nobel prize in physiology or medicine in 1964. He believed that hundreds of millions of years ago, primordial eukaryotes - organisms whose cells possess a nucleus and which ultimately led to all animals, plants, fungi and algae living today probably lacked the full sterol biosynthetic pathway. Instead, he suggested they likely generated ancestral intermediates that he dubbed 'ursterols',



JUN. 16, 2023

No need for aqua regia, chlorine or mercury in this gold processing method

Bulletin Board

Gossip

JUN. 16, 2023

which he suggested were fully adapted end products that evolved towards modern steroids.

Chemistry World, 13 June 2023

https://chemistryworld

Atomic force microscopy probes mechanochemical kinetics

2023-06-13

Experiments probing how force accelerates chemical reactions have provided new insights into mechanochemical kinetics. The findings by USbased scientists could inform the development of chemical manufacturing methods that are more sustainable and less wasteful than current approaches.

In mechanically activated organic chemistry, force drives the making and breaking of covalent bonds. This helps to minimise the waste and energy cost associated with organic synthesis because the reactions are run neat or with minimal solvent, and energy is provided through mechanical, rather than thermal, means.

Chemistry World, 13 June 2023

https://chemistryworld

Exerting force in one direction increases **Diels-Alder reactants'** sensitivity to pressure 1000 times

Curiosities

CHEMWATCH

Photosynthesis starts with a single photon, study shows 2023-06-14

The discovery solidifies our current understanding of photosynthesis and will help answer questions about how life works on the smallest of scales, where quantum physics and biology meet.

"A huge amount of work, theoretically and experimentally, has been done around the world trying to understand what happens after a photon is absorbed. But we realized that nobody was talking about the first step. That was still a question that needed to be answered in detail," said co-lead author Graham Fleming, a senior faculty scientist in the Biosciences Area at Lawrence Berkeley National Laboratory (Berkeley Lab) and professor of chemistry at UC Berkeley.

In their study, Fleming, co-lead author Birgitta Whaley, a senior faculty scientist in the Energy Sciences Area at Berkeley Lab, and their research groups showed that a single photon can indeed initiate the first step of photosynthesis in photosynthetic purple bacteria. Because all photosynthetic organisms use similar processes and share an evolutionary ancestor, the team is confident that photosynthesis in plants and algae works the same way. "Nature invented a very clever trick," Fleming said.

How living systems use light

Based on how efficient photosynthesis is at converting sunlight into energy-rich molecules, scientists have long assumed that a single photon was all it took to initiate the reaction, wherein photons pass energy to electrons that then trade places with electrons in different molecules, eventually creating the precursor ingredients for the production of sugars. After all, the sun doesn't provide that many photons—only a thousand photons arrive at a single chlorophyll molecule per second on a sunny day—yet the process occurs reliably across the planet.

However, "no one had ever backed up that assumption with a demonstration," said first author Quanwei Li, a joint postdoctoral researcher who develops new experimental techniques with quantum light in the Fleming and Whaley groups.

And, further complicating matters, a great deal of the research that has unraveled precise details about later steps of photosynthesis was performed by triggering photosynthetic molecules with powerful, ultrafast laser pulses.



Using a complex cast of metal-studded pigments, proteins, enzymes, and co-enzymes, photosynthetic organisms can convert the energy in light into the chemical energy for life. And now, thanks to a study published June 14 in Nature, we know that this organic chemical reaction is sensitive to the smallest quantity of light possible—a single photon.

Bulletin Board

Curiosities

"There's a huge difference in intensity between a laser and sunlight—a typical focused laser beam is a million times brighter than sunlight," said Li. Even if you manage to produce a weak beam with an intensity matching that of sunlight, they are still very different due to quantum properties of light called photon statistics. Since no one has seen the photon get absorbed, we don't know what difference it makes what kind of photon it is, he explained. "But just like you need to understand each particle to build a quantum computer, we need to study the quantum properties of living systems to truly understand them, and to make efficient artificial systems that generate renewable fuels."

Photosynthesis, like other chemical reactions, was first understood in bulk—meaning that we knew what the overall inputs and outputs were, and from that we could infer what interactions between individual molecules might look like. In the 1970s and 80s, advances in technology allowed scientists to directly study individual chemicals during reactions. Now, scientists are beginning to explore the next frontier, the individual atom and subatomic particle scale, using even more advanced technologies.

From assumption to fact

Designing an experiment that would allow for observation of individual photons meant bringing together a unique team of theorists and experimentalists who combined cutting-edge tools from quantum optics and biology. "It was new for people who study photosynthesis, because they don't normally use these tools, and it was new for people in guantum optics because we don't normally think about applying these techniques to complex biological systems," said Whaley, who is also a professor of chemical physics at UC Berkeley.

The scientists set up a photon source that generates a single pair of photons through a process called spontaneous parametric downconversion. During each pulse, the first photon—"the herald"—was observed with a highly sensitive detector, which confirmed that the second photon was on its way to the assembled sample of light absorbing molecular structures taken from photosynthetic bacteria. Another photon detector near the sample was set up to measure the lower-energy photon that is emitted by the photosynthetic structure after it absorbed the second "heralded" photon of the original pair.

The light absorbing structure used in the experiment, called the LH2, has been studied extensively. It is known that photons at the 800 nanometer (nm) wavelength get absorbed by a ring of nine bacteriochlorophyll

Curiosities

JUN. 16, 2023

CHEMWATCH

molecules in LH2, causing energy to be passed to a second ring of 18 bacteriochlorophyll molecules which can emit fluorescent photons at 850 nm. In the native bacteria, the energy from the photons would continue transferring to subsequent molecules until it is used to initiate the chemistry of photosynthesis. But in the experiment, when the LH2s had been separated from other cellular machinery, the detection of the 850 nm photon served as definitive sign that the process had been activated.

"If you've only got one photon, it's awfully easy to lose it. So that was the fundamental difficulty in this experiment and that's why we use the herald photon," said Fleming. The scientists analyzed more than 17.7 billion herald photon detection events and 1.6 million heralded fluorescent photon detection events to ensure that the observations could only be attributed to single-photon absorption, and that no other factors were influencing the results.

"I think the first thing is that this experiment has shown that you can actually do things with individual photons. So that's a very, very important point," said Whaley. "The next thing is, what else can we do? Our goal is to study the energy transfer from individual photons through the photosynthetic complex at the shortest possible temporal and spatial scales."

Phys Org, 14 June 2023

https://phys.org

Researchers report light-controlled transport of biomolecules across the cell membrane 2023-06-14

In collaboration with a team from the Universidade Nova de Lisboa (NOVA), researchers from the Center for Research in Biological Chemistry and Molecular Materials (CiQUS) at University of Santiago de Compostela reported new light-responsive membrane transporters for the translocation of peptide cargos inside living cells.

"Our design relied on calixarene-based receptors with an azobenzene unit that can be applied as photoresponsive counterion to gain control over the transport of cationic peptides," said Prof. Javier Montenegro, Principal Investigator at CiQUS. Counterions are oppositely charged ions that are attracted to the charged compound, forming charge-neutralized complexes with higher membrane permeability in this case.

Bulletin Board

JUN. 16, 2023

Crossing the membrane is a major challenge on the journey through the cell. Large biomolecules usually benefit from different transport strategies to overcome the lipid bilayer, so the design and synthesis of new carriers is key for the delivery of hydrophilic substances, such as pharmaceuticals, into the cell. Among these transporters, those using light as stimulus are particularly appealing due to their high precision, no chemical waste production and the possibility of remote application.

Bulletin Board

Curiosities

When light irradiated, azobenzenes units change their configuration from a more polar to a more hydrophobic conformation, successfully making their way into the cytosol. "The dynamic control of the structure and polarity of counterion activators by using light offers a promising conceptual strategy to develop stimuli responsive membrane carriers," explained Dr. Nuno Basílio, researcher at NOVA and co-author of the work recently published in the Journal of the American Chemical Society (JACS).

According to the authors, the synthesis of such molecular photoswitches shows their potential for the light-triggered delivery of large biomolecules and envisage new possibilities in remotely controlled systems for pharmaceutical applications.

Phys Org, 14 June 2023

https://phys.org

Scientists develop novel biosensing-membrane for glucose detection and monitoring 2023-06-14

The glucose oxidase/electrocatalysts/electrode (GOx/ECs/electrode) cascade system serves as the core part of most glucose biosensing devices (both invasive and non-invasive). However, patterned assembly of these cascade sensing units remains challenging, thus limiting the attainment of high sensitivity and long-term stability.

Inspired by the structure of electron-transfer chains in the mitochondria, a research group led by Prof. Wan Yinhua from the Institute of Process Engineering (IPE) of the Chinese Academy of Sciences has developed a three-dimensional (3D) mesoporous biosensing-membrane with neighborhood nanostructures that shows excellent sensitivity and longterm stability.

The study was published in Advanced Functional Materials.

In preparing the biosensing-membranes, the researchers used tannic acid-3-aminopropyltriethoxysilane-Fe3+ (TA-APTES-Fe) ternary coating to properly assemble and adjacently confine Prussian blue (PB) and GOx in the 3D mesoporous carbon nanotube (CNT) membrane electrode.

"This strategy enhances the cascade sensing units with close proximity and extends the triple-phase boundary (TPB) from conventional 2D contact to 3D contact, which boosts the cascade reaction efficiency,

Glucose oxidase (GOx)-based biosensors have attracted much attention for their potential in rapid glucose detection and continuous monitoring, which are crucial for disease diagnosis and prevention, as well as for controllable production in sugar-making and fermentation processes.

JUN. 16, 2023

Curiosities

CHEMWATCH

improves the accessibility and availability of H2O2 toward the TPB, and increases the utilization of PB," said Prof. Luo Jianguan from IPE.

Moreover, the spatially confined microenvironment stabilizes PB and GOx. The separation function of the CNT membrane further intensifies the sensing stability by in-situ removal of interferents from the analytes.

The as-prepared mesoporous biosensing-membrane exhibits good sensitivity and long-term stability with a negligible response drift for up to eight hours, thus outperforming the reported results.

"The multienzyme mimic functions of PB have been employed to imitate the 'loosening-degradation' membrane cleaning process, fully regenerating the fouled biosensing-membrane," said Prof. Wan.

This work provides a novel design and operation strategy for biosensors, ensuring efficient, reliable, and stable sensing.

Phys Org, 14 June 2023

https://phys.org

New research provides a rapid and non-destructive method for identifying honey's botanical origin 2023-06-14

The study, published in the Journal of Food Composition and Analysis, successfully demonstrates a workflow to swiftly identify the botanical origin of honey, a task that has traditionally necessitated extensive highend analysis.

Honey's botanical origin influences not only its market price but also its organoleptic properties and potential health benefits, making it a critical factor in consumer choice. This breakthrough comes as a boon to industry stakeholders, who can now categorize honey in a more precise and costeffective manner.

Indicative FTIR spectra for each of the analyzed honey matrices. Each color represents a different matrix as it is displayed in the legend. Credit: Journal of Food Composition and Analysis (2023). DOI: 10.1016/j.jfca.2023.105276

The researchers tested 22 different pre-processing methods and combinations, including scatter correction methods and spectral derivation methods, using both supervised and non-supervised tools. Their efforts revolved around optimally projecting a diverse array of 51



JUN. 16, 2023

Researchers at the University of **Chemistry and Tech**nology in Prague have developed a rapid, non-destructive method using attenuated total reflectance **Fourier transform** infrared spectroscopy (ATR-FTIR) to identify the botanical origin of honey. This method, which efficiently categorizes honey based on origin, has implications for honey pricing and marketability, aiding in more precise and cost-effective product differentiation.

Bulletin Board

Curiosities

honey samples from five different botanical origins: blossom, honeydew, cotton, thyme, and citrus.

The study's pivotal finding suggests the most efficient data pre-processing method is the combination of multiplicative scatter correction followed by Savitzky-Golay first derivation. This procedure resulted in excellent recognition (87–100%) and prediction (81–100%) ability when applied in binary models.

The findings highlight the significant yet often overlooked effect of spectral data pre-processing before the application of advanced chemometrics. This novel approach will pave the way for rapid and efficient identification of honey's botanical origin, thereby providing a much-needed enhancement in the world of honey production and marketing.

Phys Org, 14 June 2023

https://phys.org

Light and nickel found to simplify cross-coupling reactions

2023-06-14

Given the numerous factors that can affect the outcome of the reaction, such as the presence or absence of ligand molecules, catalyst precursors, bases, and other additives, optimization is a tedious task. Machine learning and artificial intelligence are promising new approaches to predicting optimal reaction conditions, but training such models also involves significant effort.

A solution to this problem that has now been found by researchers at the University of Regensburg (UR) in cooperation with the Zelinisky Institute in Moscow takes a completely different approach: the reaction parameters have been reduced to a minimum and only the two reaction partners that are to be linked are combined with a simple nickel salt and an organic dye under exposure to visible light.

No traditional ligands or additives are added to constrain the nickel catalyst (i.e., they provide multiple channels for catalytic reactivity), as is the case in most conventional methods. Under the reaction conditions, a dynamic mixture of many metal complexes is formed, whose electronic state is adjusted by the photocatalyst and the absorbed light energy in such a way that catalytic reactions begin.

Cross-coupling reactions—chemical transformations in which two fragments are joined together—are a valuable tool in the synthesis of organic molecules. Applications range from drug development and synthesis of naturally occurring molecules to materials science. **Despite many known** methods, finding the right conditions for new reactions remained a challenge.

JUN. 16, 2023

Curiosities

CHEMWATCH

The principle is comparable to a juggling feat; through which the photocatalyst and the light energy repeatedly bring metal complexes into the catalytically active form, like throwing balls up when juggling. Since light energy is only required to activate the catalysts and these are very reactive without stabilization, energy-efficient, fast reactions are possible.

Catalysts that lose their activity (in the juggling feat, these are dropped balls) are continuously repaired by the light energy, so that only extremely small amounts of the catalyst metal, nickel, are needed. The results of years of research have now been published in Nature.

It was possible to identify reaction conditions for all molecule classes that now allow reliable planning of syntheses. The new reaction principle is referred to as Adaptive Dynamic HOmogeneous Catalysis, or AD-HoC for short, and makes an important contribution to the development of energy-efficient and effective, and therefore more sustainable, chemical reactions.

The project has been running for about three years. During this time, numerous experiments were conducted to further develop and confirm the central discovery. The systematic classification of reactants was a breakthrough moment and a particular analytical method of the Russian collaborators, in-situ-mass-spectrometry, helped to understand the dynamic nature of the catalytic systems.

In future work, the concept will now be extended to other metal ions such as copper, cobalt, or iron, and other types of reactions, such as the activation of carbon-hydrogen bonds.

Furthermore, the researchers believe that the predictability of the reaction conditions together with the simplicity and efficiency will allow this method to be used in industry either for the synthesis of active pharmaceutical ingredients (APIs), which normally requires a time-consuming series of optimization steps, or for the functionalization of biomolecules or for energy-efficient synthetic transformations on a large scale.

Phys Org, 14 June 2023

https://phys.org

Bulletin Board

JUN. 16, 2023

Food waste and food-borne diseases are among the most critical problems urban populations face today. They contribute to greenhouse emissions tremendously and amplify economic and environmental costs. Since food spoilage remains the main reason for this waste, the circumstances of processing, transporting, and preserving food still need to be improved in line with current technological advancements.

Bulletin Board

Curiosities

JUN. 16, 2023

Wireless sensor enables real-time spoilage alerts on food

2023-06-09

Current monitoring processes are conducted in laboratories and use expensive chromatographic devices. These not only require too much time but also excessive resources and gualified personnel. So, present methods unfortunately prove to be inefficient in today's circumstances.

New research published in Nature Food presents a significant alternative to this process: A new user-friendly, cost-effective, and up-to-date sensor that can be applied on food directly and replace lab-monitoring. The 2 x 2 cm miniature wireless device introduced in the paper offers real-time measurement, is battery-free and smartphone-compatible. It is expected to be highly effective especially in high-protein foods such as beef, chicken, and fish.

The research was led by Dr. Emin İstif (Molecular Biology and Genetics, Kadir Has University) and Asst. Prof. Levent Beker (Mechanical Engineering, Koc University) with the contribution of Prof. İskender Yılgör and Dr. Emel Yılgör (Chemistry, Koç University), Asst. Prof. Çağdaş Dağ (Molecular Biology and Genetics, Koc University) and Asst Prof. Hatice Ceylan Koydemir (Texas A&M University).

While existing solutions focus on the change in color of food, this new device, for the first time, offers a capacitive measurement method and thus utilizes near-field communication (NFC) technology with power-free and wireless communication. The authors indicate that this eliminates major disadvantages encountered in resistive devices such as moisture sensitivity and incorrect data due to distance.

The invention will not only provide companies the opportunity of reducing costs but also help consumers tremendously. Once widely commercialized, the device will enable continuous monitoring on shelves and allow users to control freshness right before buying a product or even before consumption at home. This opportunity of on-demand spoilage analysis via mobile phones will ultimately help preventing food waste and food-borne diseases.

With its cost-effectiveness and accessibility, the authors hope to contribute to the greater struggle against global warming and greenhouse emissions

Curiosities

CHEMWATCH

more effectively and quickly. The next steps will be to focus on increasing the potential for commercialization of the product in the near future.

Phys Org, 9 June 2023

https://phys.org

A conductive self-healing hydrogel to create flexible sensors

2023-06-02

While material scientists have already introduced a wide range of flexible materials that could be used to create electronics, many of these materials are fragile and can be easily damaged. As damage to materials can result in their failure, while also compromising the overall functioning of the system they are integrated in, several existing soft and conductive materials can end up being unreliable and unsuitable for large-scale implementations.

Researchers at Harbin University of Science and Technology in China recently developed a new conductive and self-healing hydrogel that could be used to create flexible sensors for wearables, robots or other devices. This material and its composition was outlined in the Journal of Science: Advanced Materials and Devices.

"In this paper, polyvinyl alcohol (PVA) and 4-carboxylbenzaldehyde (CBA) were used to form a double network skeleton, and polyaniline (PANI) was introduced to assemble a flexible sensor with excellent self-healing performance," Xiaoming Wang, Ling Weng and their colleagues wrote in their paper. "The hydrophobic association of PVA and CBA guarantees the mechanical properties of the hydrogel sensor, and the introduction of PANI brings electrical properties to the hydrogel sensor."

Wang, Weng and their colleagues created their material by introducing CBA, an organic compound consisting of a benzene ring substituted with an aldehyde and carboxylic acid, into PVA, a water-soluble synthetic polymer, and adding the conducting polymer PANI via an electrostatic interaction. In initial tests, they found that the material had remarkable mechanical properties and could heal itself after being damaged. Moreover, it could reach a maximum stress of 4.35 Mpa and a maximum strain of 380%.

The researchers then used the material to create a strain sensor, a sensing device that can detect external forces and applied pressure originating



Recent advancements in the field of electronics have enabled the creation of smaller and increasingly sophisticated devices, including wearable technologies, biosensors, medical implants, and soft robots. Most of these technologies are based on stretchy materials with electronic properties.

Bulletin Board

Curiosities

from its surroundings. This sensor was found to perform very well, measuring both small deformation signals, such as a wearer coughing or speaking, as well as more vigorous body movements.

"The flexible sensor prepared in this article has a sensitivity of 1.71 in the strain range of 0-300%, and a limit detection strain of less than 1%," Wang, Weng and their colleagues wrote in their paper. "The response time of the hydrogel sensor during stretching is 158 ms. In addition, the hydrogel sensor also has self-healing performance. At room temperature, after the hydrogel is cut, it only takes one min to complete the repair, and the selfhealing rate is about 60%."

In the future, the hydrogel created by this team of researchers could be used to develop a wide range of other sensors and wearable electronics, such as sensors that can detect human motion or medical devices that monitor specific biological signals. In addition, their work could pave the way for the development of similar flexible and conductive hydrogels with self-healing properties.

Phys Org, 2 June 2023

https://phys.org

Buckle up: A new class of materials is here 2023-06-02

A team of researchers from the University of Amsterdam has now found a way to create materials that are stiff, but still good at absorbing vibrations—and equally importantly, that can be kept very light-weight.

David Dykstra, lead author of the study published in the journal Advanced Materials, explains, "We discovered that the trick was to use materials that buckle, like thin metal sheets. When put together in a clever way, constructions made out of such buckled sheets become great absorbers of vibrations—but at the same time, they preserve a lot of the stiffness of the material they are made out of. Moreover, the sheets do not need to be very thick, and so the material can be kept relatively light."

The researchers thoroughly investigated the properties of these buckled materials, and found that they all showed this magical combination of stiffness and ability to dissipate vibrations. As known materials do not have this desired combination of properties, the new lab-made materials (or metamaterials) have a very wide range of potential applications, and at a very wide range of scales.

Usually, the two characterizations of a material are mutually exclusive: something is either stiff, or it can absorb vibrations well—but rarely both. However, if we could make materials that are both stiff and good at absorbing vibrations, there would be a whole host of potential applications, from design at the nanoscale to aerospace engineering.

JUN. 16, 2023

Curiosities

CHEMWATCH

Possible uses range from meter-sized (think of aerospace, automotive applications and many other civil designs) to the microscale (applications such as microscopes or nanolithography).

Dykstra says, "Humans like to build things—small things and big things and we almost always want these structures to be light. If that can be done with materials that are both stiff and good at shock-absorbing, many existing designs can be improved and many new designs become possible. There really is no end to the possible applications."

Phys Org, 2 June 2023

https://phys.org

Scientists create fluorogenic probe to detect enzyme linked to early stage of Alzheimer's 2023-06-14

"Our goal was to find a reliable, cost-effective solution," says Debasis Das, Assistant Professor in the Department of Inorganic and Physical Chemistry (IPC), Indian Institute of Science (IISc). In a study published in Analytical Chemistry, he and Jagpreet Sidhu, a CV Raman postdoctoral fellow in IPC, have designed a small molecular fluorogenic probe that can sense a specific enzyme linked to the progression of Alzheimer's disease. Such a probe can easily be fabricated into a strip-based kit that may enable onsite diagnosis.

"Fluorogenic probes are not fluorescent by themselves, but upon reaction with a target enzyme, they become fluorescent," explains Das. "Our target enzyme is Acetylcholinesterase (AChE)." Studies have shown that in the early stages of Alzheimer's disease, AChE levels become imbalanced, thus making it a potential biomarker for the disease.

Brain cells or neurons secrete neurotransmitters—signaling molecules that instruct other cells to perform certain functions. Acetylcholine (ACh) is one such neurotransmitter; its levels in our nervous system are tightly controlled by enzymes like AChE, which breaks it down into two parts—acetic acid and choline. Current approaches determine AChE levels indirectly by measuring the levels of choline. They also often give confounding results because AChE has "sister enzymes" such as butyrylcholinesterase and cholinesterase that work on similar substrates, including ACh, says Das.



Alzheimer's disease, a neurodegenerative disorder, results in memory loss and compromises cognitive abilities in many people beyond the age of 60. Currently used techniques to detect manifestations of the disease (MRI, PET, and CT scans) are complex, expensive and often produce inconclusive results.

Bulletin Board

Curiosities

The team first analyzed the crystal structures of the enzyme (AChE) and the substrate (ACh). Then, they designed a synthetic molecule that mimics ACh. The probe developed by the team has one structural element (quaternary ammonium) that interacts specifically with AChE, and another that binds to the active site in AChE and gets digested (just like natural ACh), giving out a fluorescent signal. The team tweaked the distance between the two elements to make it bind tightly to the enzyme."In previous reports, people did not use this quaternary ammonium group. Because of this, they were not able to attain specificity and selectivity," says Sidhu, who is the first author of the study.

To test the probe's ability to be digested specifically by the enzyme, the team used commercially available AChE as well as lab-made human brain AChE expressed in bacteria. Although AChE has been extracted from the human brain, purified, and crystallized in the past, this is the first time that it has been purified in the active form after cloning and expressing it in a bacterial system, the researchers say.

In collaboration with Deepak Saini's lab at the Department of Developmental Biology and Genetics, IISc, the team showed that the fluorogenic probe could also enter brain cells cultured in the lab and fluoresce upon contact with AChE.

"We now have a proof-of-concept and a lead. Our goal is to take it to translation, in an Alzheimer's disease model. For this, we need to modify the probe," says Das. Currently, the probe is UV-active, which can be harmful to tissues in high doses. "These modifications would lead to the development of near-infrared active probes, which would be safer for living cells and allow deep-tissue imaging. We are already quite close to doing this."

Apart from Alzheimer's disease, such a probe can also be used for other applications like detecting pesticide-related poisoning, as AChE can be inhibited by compounds used in some pesticides, Sidhu adds.

Phys Org, 14 June 2023

https://phys.org

Stimuli-responsive fluorescent hydrogels (FHs) are excellent and attractive candidates for information encryption and anticounterfeiting applications, which can allow the stored information to be visualized by a vibrant display with a higher degree of security levels. However, hydrogelbased information storage devices for anti-counterfeiting are still in their infancy, so developing an environment-friendly, low-cost, and scalable approach to produce stimuli-responsive FHs is still challenging.

JUN. 16, 2023

CHEMWATCH

Bulletin Board

Curiosities

New strategy using curcumin provides smart fluorescence for anti-counterfeiting 2023-06-13

Curcumin is a natural biocompatible and sustainable material, which has shown great therapeutic potential as an anti-diabetic, anti-inflammatory, and anti-cancer compound. Although it is a pH-sensitive and fluorescent molecule, it is difficult to use in the hydrogels as fluorescent agent due to its very weak fluorescence in polar water.

A study published in Green Chemical Engineering has introduced a new strategy to construct strong fluorescent hydrogels using curcumin as a fluorescent agent. The curcumin was loaded in to an amphiphilic quaternary ammonium (QA) micelle, which endows the hydrogels with excellent mechanical properties and both pH-responsive color and fluorescence to provide a dual anti-counterfeiting capability.

This facile scalable method for fabricating the pH-FHs shows great potential for producing materials for information encryption and anticounterfeiting applications.

Co-corresponding author Xiubin Xu, from the School of Chemistry and Chemical Engineering of Guangzhou University in China, explains, "Compared to conventional fluorescent agents, curcumin is natural, biocompatible, and sustainable, which is meaningful and interesting to facilitate its scalable application, such as anti-counterfeiting. As a result, we were able to obtain fluorescent hydrogels using the curcumin as fluorescent agents, which shows good mechanical properties, good antifatigue performance, and smart fluorescence responding to ammonia gas and formaldehyde gas."

"The hydrogels also exhibit information storage-rewriting behavior and dual anti-counterfeiting capabilities. We believe that these strategies and achievements can facilitate the design of robust and smart FHs for information encryption and anti-counterfeiting applications."

PhyS Org, 13 June 2023

https://phys.org





Technical Notes

(NOTE: OPEN YOUR WEB BROWSER AND CLICK ON HEADING TO LINK TO SECTION)

JUN. 16, 2023

-40

CHEMICAL EFFECTS

Bioenergy Generation and Phenol Degradation through Microbial Fuel Cells Energized by Domestic Organic Waste

ENVIRONMENTAL RESEARCH

Distributed IoT Air Quality Measurement System for High-Risk Workplace Safety Enhancement

An updated global overview of the manufacture and unintentional formation of polychlorinated naphthalenes (PCNs)

Sunlight and marine weathering of poly(oxymethylene): Evolution of the physico-chemical properties

Performance and Mechanism of Chlorine Dioxide on BTEX Removal in Liquid and Indoor Air

PHARMACEUTICAL/TOXICOLOGY

Cancer incidence among workers in soft paper mills: A cohort study

Assessing the chemical composition, potential toxicity and cancer risk of airborne fine particulate matter (PM2.5) near a petrochemical industrial area

OCCUPATIONAL

Work in nursing homes and occupational exposure to endotoxin and bacterial and fungal species

The Epidemiological Surveillance of Mesothelioma Mortality in Italy as a Tool for the Prevention of Asbestos Exposure

Distributed IoT Air Quality Measurement System for High-Risk Workplace Safety Enhancement