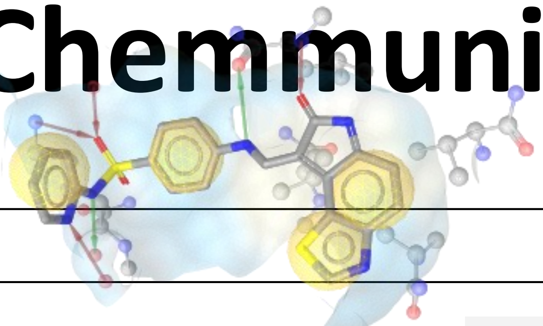
Chemmuniqué



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Dean's Message

It is an immense pleasure to note that the newsletter *Chemmuniqué* being brought out by the Department of Chemistry will be released as the fifth volume. Hearty congratulations to the editorial team! The newsletter is an opportunity for the budding writers to explore and expand their horizon in the scientific arena under the guidance of learned teachers. Through this, students as well as teachers are exposed to a variety of important and interesting developments in different areas around the world. Such activities will enhance the quality of education and thus enrich intellectual skills of the young talents.

-N.M.Nanjegowda

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Lighting up the field of Cancer Diagnostics

Move away cumbersome and expensive techniques of cancer detection, for entering the arena is the all-new, safer, simpler and cheaper way of doing so - Firefly light! Who would have thought that something as simple as the firefly could give us a simple solution to one of the most pressing problems in the pharmaceutical industry?

Researchers at the EPFL labs, Switzerland (École polytechnique fédérale de Lausanne) have recently devised a technique of extracting luciferase, the enzyme which gives fireflies its characteristic light and using it to detect tumors or target molecules within a living system. While initially trials were conducted to locate the protein Streptavidin (which, in this case, is called an effector protein), scientists Alberto Schena and Rudolf Griss, firmly believe that this principle can be extended to create biosensors for all kinds of biomolecules and tumor cells.

The experiment involved first synthesizing a dual ligand containing luciferase inhibitor 'Coelenteramide' and an artificially synthesized ligand of Streptavidin called Biotin. Using the help of a chemical tag, the dual ligand is then bound to the enzyme. In the absence of the effector protein, Coelenteramide inhibits the activity of luciferase and prevents it from illuminating. However, once the Streptavidin is detected, it binds to biotin because of which the inhibitor is signaled to eject the enzyme and finally activate it. Once in the active state, it begins emitting light at an intensity that was found to be greater than 1,700 times the original intensity, thus allowing it to be detected even by the naked eye.

With advancements in this technology and synthesizing different binders to detect different proteins of interest, it would not be a surprise if the current state of medical diagnostics in the world changes for the better, making the system of disease detection more efficient, safer and cheaper in the near future.

DALIA JANE SALDANHA, II BCZ

Editorial

It is exactly 100 years since man first used the chemical weapon; in 1915 during the First World War. Fritz Haber the German scientist, who had earlier proposed using chlorine gas on Allied troops and overseen its development as a weapon, had gone to the front lines himself to supervise placement of 5,730 gas cylinders along a 4-mile stretch of road near the trenches outside the Belgian town of Ypres. The first large-scale use of chemical weapons that day in 1915 ignited a chemical arms race among the warring parties. By the end of World War I, scientists working for both sides had evaluated some 3,000 different chemicals for use as possible weapons; around 50 of these poisons were actually tried out on the battlefield. The image of chemistry took a beating it is still trying to recover from. Over the subsequent decades, Chemistry has contributed immensely to the welfare of humankind: pharmaceutical drugs, fertilizers, insecticides and pesticides to name but a few. The tainted image of chemistry and the chemical industry persists, so how can the industry and chemists move forward? Many people believe the answer lies in good communication and education. Newsletters like Chémmuniqué are a small step in that direction.

World of Ionic Liquids!

Hello! Welcome to our world. A world obscure to most of the budding chemists. Nevertheless, we have prompted multi-dimensional researches, owing to our dynamic physiochemical properties, versatile applications and promising environment friendly behavior.

We are a broad class of ionic compounds, mostly having melting points below ŏ C and high boiling points. We are organic salts - cations are organic, while anions may be organic or inorganic. Interactions between the ions are mostly columbic in nature.

The best thing about us is that we have *tunable properties*. Our properties can be incredibly varied by just altering the combination of cations and anions. This gives us the name of “designer liquids”. 10^{18} ionic liquids can be tailored using various permutation and combinations of cations and anions.

We have unconventionally low melting points (liquid at room temperature), temptingly negligible vapour pressure, variable miscibility, conductivity (solely composed of ions), appreciably wide electrochemical window and high thermal stability.

We are often referred to as “*green solvents*” as we hold the potential to replace volatile, toxic, hazardous organic solvents as an alternative (mainly due to low vapour pressure). We are fluid over a broad temperature range, safer to work with as we are mostly non-inflammable and non-explosive (in nature).

We have a variety of electrolytic applications – in batteries, capacitors and solar cells, electrochemical processes, metal extraction, separation, extraction, electro analysis, sensing and spectrometry is noteworthy. We serve as a good medium to solubilize gases such as H_2, CO, O_2 and CO_2. Our biocompatible nature has opened doors for use in pharmaceutical industries for enzymatic reactions, DNA and protein solubilization. We have emerged as a potential replacement for organic solvents in biocatalytic processes both at laboratory and industrial scale.

Many classes of chemical reactions, such as Diels-Alder reactions and Friedel-Crafts reactions, can be performed using ionic liquids as solvents.

Further exploration would let the world realize the abundance of potential we hold in satisfying modern days’ needs through our versatile nature. J

SAGARIKA MISHRA, II M.Sc

THE CONFEDERATE ROSE

INTRODUCTION

Hibiscus mutabilis or the **confederate rose** or **cotton rosemallow** is known for its salient property of exhibiting various colours during its life cycle. It belongs to the botanical family *Malvacea.* It is a native of Southern China and the Confederate State of America and is cultivated in the Indian sub-continent for its floral pulchritude. Flowers can be double or single and are 4 to 6 inches in diameter. They open white, gradually change to pink, and change to deep red by evening. The red flowers remain on plants for several days before they abort. This conspicuous feature was studied by various botanists and phytochemists, which led to the unveiling of its chemical background. Certain pharma properties were also discovered.

PHYTOCHEMISTRY

On flowering it exhibits a white colour which gradually changes into pink due to presence of **anthocyanin** in the vacuoles of the petals, whose synthesis occurs at low temperatures (around 293K). This chemical is a vital component in the catalysis of the conversion of colourless **leuco anthocyanidin** (responsible for white colour of the flower) into **anthocyanidin** (responsible for the pink and red colours of the flower). This reaction requires low temperatures such as 293K and pH ranging from 5 to 7. It is a complex reaction involving the following steps.

The above image shows the gradual change of the colour from completely white to a shade of dark pink.

PHARMACOLOGICAL PROPERTIES

On studying the biochemistry of the flower, its pharmacological significance also came into light. The leaves and roots of this plant were found to be edible. The leaves are reported to have anodyne, antidotal, demulcent, expectorant and refrigerant properties. This part is also used for burns, pectoral and pulmonary complaints, swellings and other skin problems. A decoction of the flowers is used in the treatment of lung ailments. This plant is recommended for persistent cough, menorrhagia, dysuria and wound caused by burn and scalds. It contain large amount of mucilage which would act as emollient for burns. Inflammation is treated by the plant. The plant has been reported as a remedy for cancer. The above listed pharmacological aspects of this plant has been a great discovery in the fields of biochemistry and pharmacology.

CONCLUSION

This flower was studied extensively for its biochemical properties which had not only lead to the discovery of the phytochemistry behind the colourful mystery of the flower, but also lead to the discovery of various pharmacological aspects. To put it all in a nutshell we can simply say that this flower has ornamental as well as medicinal significance.

RISHI RAJESH, 1 BCZ

SCIENTIFIC BASIS BEHIND FOLKLORE!

Sweet grass contains a compound that can repel mosquitoes

Mosquitoes and other insects remain a pesky part of everyday life in many parts of the world. Indigenous tribes of Montana and Alberta wore braids of the sweet grass and hung it in their homes. A common folklore describes the grass to possess mosquito repellant properties.

Charles Cantrell, a research chemist who works for the US Department of Agriculture, in his research found that sweet grass (hierochloe odorata), a native of northern America gives off a sweet aroma that repels mosquitoes. Charles did steam distillation of the sweet grass and he separated oil and water.

To test the mosquitoes' aversion to the oil, he filled small vials with a red-colored feeding solution that mimicked human blood and covered the vials with a thin membrane. Then, he coated the membranes with different substances: the sweet grass oil, alternative sweet grass extracts obtained without steam distillation, the gold-standard insect repellent N,N-diethyl-m-toluamide (DEET) or the ethanol solvent control. Then, the bugs got the chance to either bite the membranes to get to the blood or pass them by. Charles Cantrell observed what the insects did; counting how many mosquitoes went for a bite of each type of "blood" vat.

Then he took the mosquitoes and crushed them on some paper. If they have the blood mimic in them, you see it right there on the paper. Of the sweet grass extracts, the steam-distilled oil got the fewest mosquito bites, matching the repellent potency of DEET (a common synthetic mosquito repellant).

Later, he figured out the exact chemicals that give the sweet grass oil its anti-mosquito power. Charles purified the oil into 12 fractions and again checked their ability to ward off the bugs. He found three fractions that repelled mosquitoes as well as the oil.

Using nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry, the researchers identified two chemicals in these active fractions that seemed to be responsible for putting off mosquitoes: phytol and coumarin.

Coumarin is an ingredient in some commercial anti-mosquito products, while phytol is reported to have repelling activity in the scientific literature. So although Cantrell didn't find brand-new insect deterrents in this experiment, he says "we were able to find constituents that are known to act as insect repellents in a folk remedy, and now we understand that there is a real scientific basis to this folklore."

ANIL KUMAR, III BCZ

Cooking Blunders: Recycling of cooking oil – a threat to our health

Food is the mantra for energy and survival that provides us with nutrition and helps us regulate growth, maintain and repair body tissues.

Although it is recommended to have a balanced diet of carbohydrates, fats and proteins yet we eventually end up consuming more fatty products owing to the irresistible taste and aroma. We all love-fried food! Potato chips, French fries, fried meat etc are our all time favorites.

Oil is an essential requirement for cooking food. Some people tend to reuse cooking oil with a false belief that it would add flavor to food and also cut down expenses. But, after reusing the oil for some time, the food starts to taste a little different and the odor of the oil also changes. This is the foul odour that we come across while passing by the roadside snack shops. This happens because the oil has become rancid.

There are different ways in which the oil can become rancid - it may undergo hydrolytic rancidity or oxidative rancidity or high temperature could affect the properties of cooking oil.

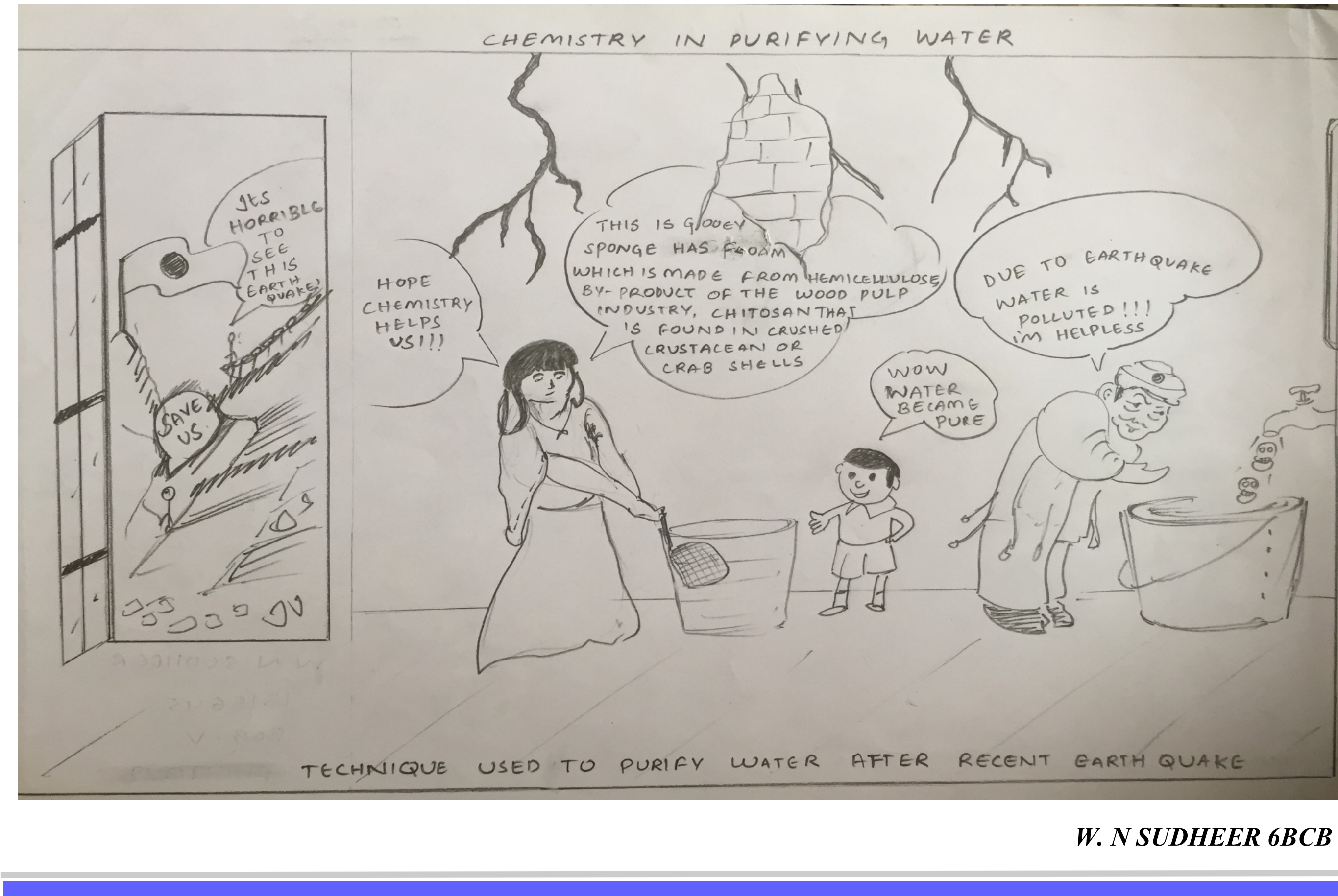
In recent researches, it was found that a toxin known as 4-hydroxy-trans-2 nonenal (HNE) forms as a result of reheating sunflower, canola, corn and soya bean oil. Consuming this toxin can lead to cardiovascular diseases, Alzheimer's, Parkinson's, heart stroke, Huntington's and various liver disorders.

Oxidative and hydrolytic rancidity of oils actually change the chemical structure of cooking oils. Oxidative rancidity leads to the formation of peroxides and then they break down to give rise to free radicals. These radicals are reactive and cause cellular damage. They damage the DNA ultimately causing cancer in the long run.

There is high acid content in oxidized oil. As a result of oxidative rancidity, there is high carboxylic acid content in the oil, thereby releasing a pungent smell. Consuming rancid oils could also accelerate ageing.

Hence, we must abstain from reusing cooking oil, as instead of cutting down on the oil expenses, it just invites us more health troubles.

DEBARATI BHOWMIK & SANGEETH SIVAN, 1 BCB

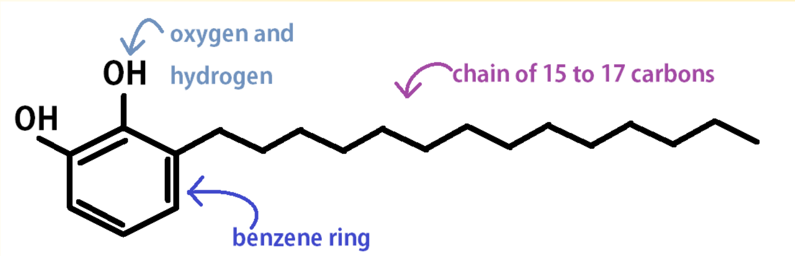


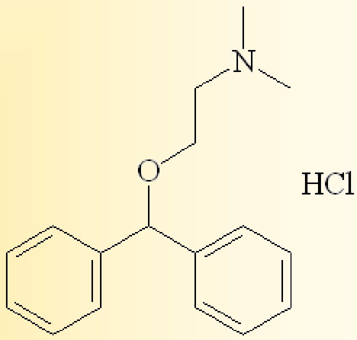
W. N SUDHEER 6BCB

POISON IVY

Poison Ivy? The beautiful and villainous adversary of Batman in the DC comic Universe. However venomous she might be among the people of Gotham, the real life Poison Ivy is no less when compared to spreading its toxic effect than the former. *Toxicodendronradicans*, a member of the family *Anacardacae* of the Plant Kingdom, is found near the Eastern Sea Shores of the United States of America. It is easily identifiable but hardly avoidable. The reason of this statement is the presence of them as a group of 3 leaflets as the saying warns "*Leaves of three, let them be.*" The leaves produce a chemical called ***Urushiol.***

Urushiol is a pro-electrophilic antigen presenting molecule. It creates an allergic reaction on the skin when in contact, leading to ***Contact Dermatitis.*** The severity of the reaction depends on the length and unsaturation of the side chain. So less the branching , more the reaction. Therefore, Urushiol V has more severe reaction than Urushiol IV.





Where the *15-17 carbon* chain can be an R group :

$R=(CH_2)_{14}CH_3$ or

$R=(CH_2)_7CH=CH(CH_2)_5CH_3$ or

$R=(CH_2)_7CH=CHCH_2CH=CH(CH_2)_2CH_3$ or

$R=(CH_2)_7CH=CHCH_2CH=CHCH=CHCH_3$ or

$R = (CH_2)_7CH=CHCH_2CH=CHCH_2CH=CH_2$and others

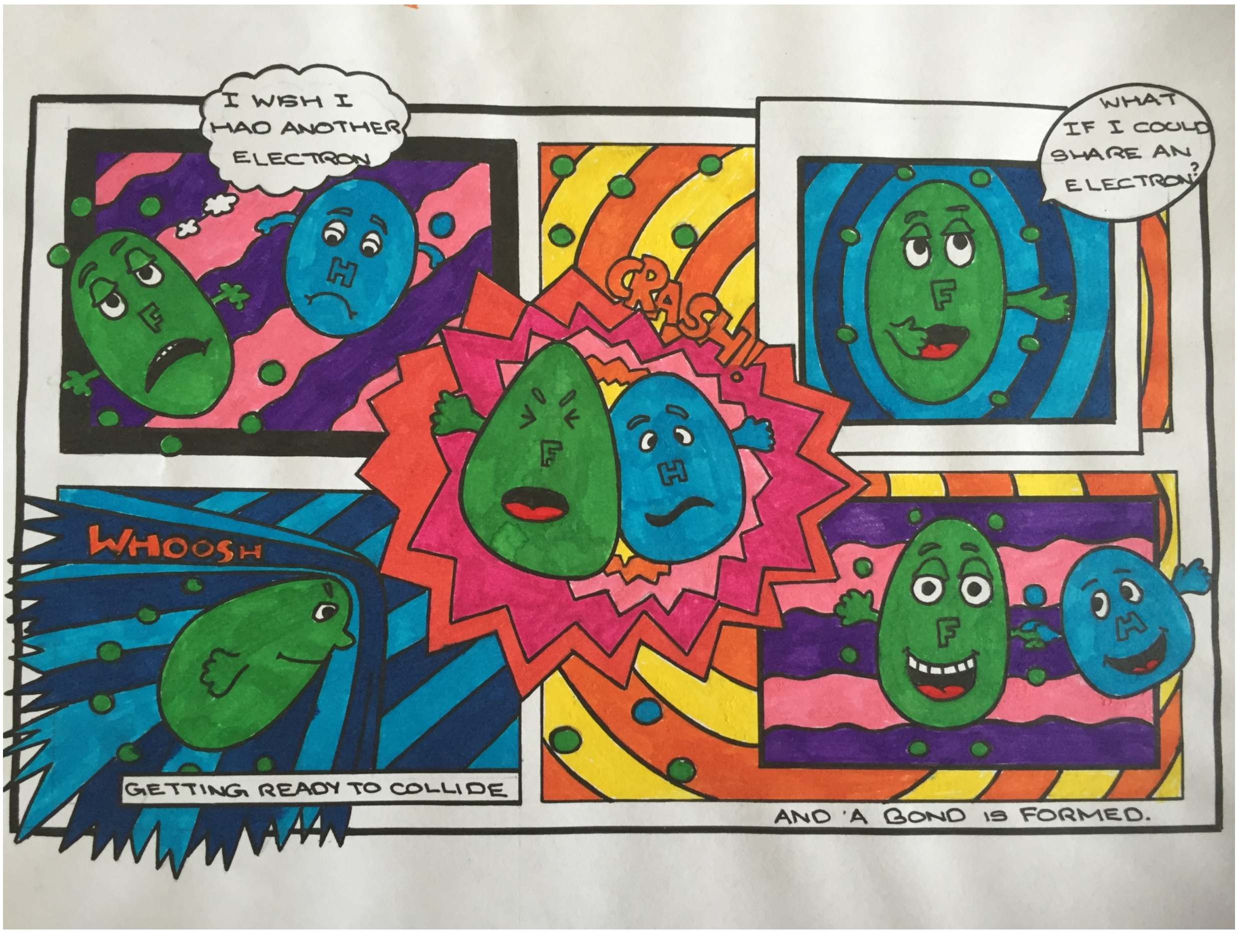
On exposure to skin, a protein complex is formed, as a result of electrophilic attack of the amino acids of the protein (act as nucleophiles). Then Urushiol is converted into a reactive ***Quinone*** (oxidised form of a catechol).

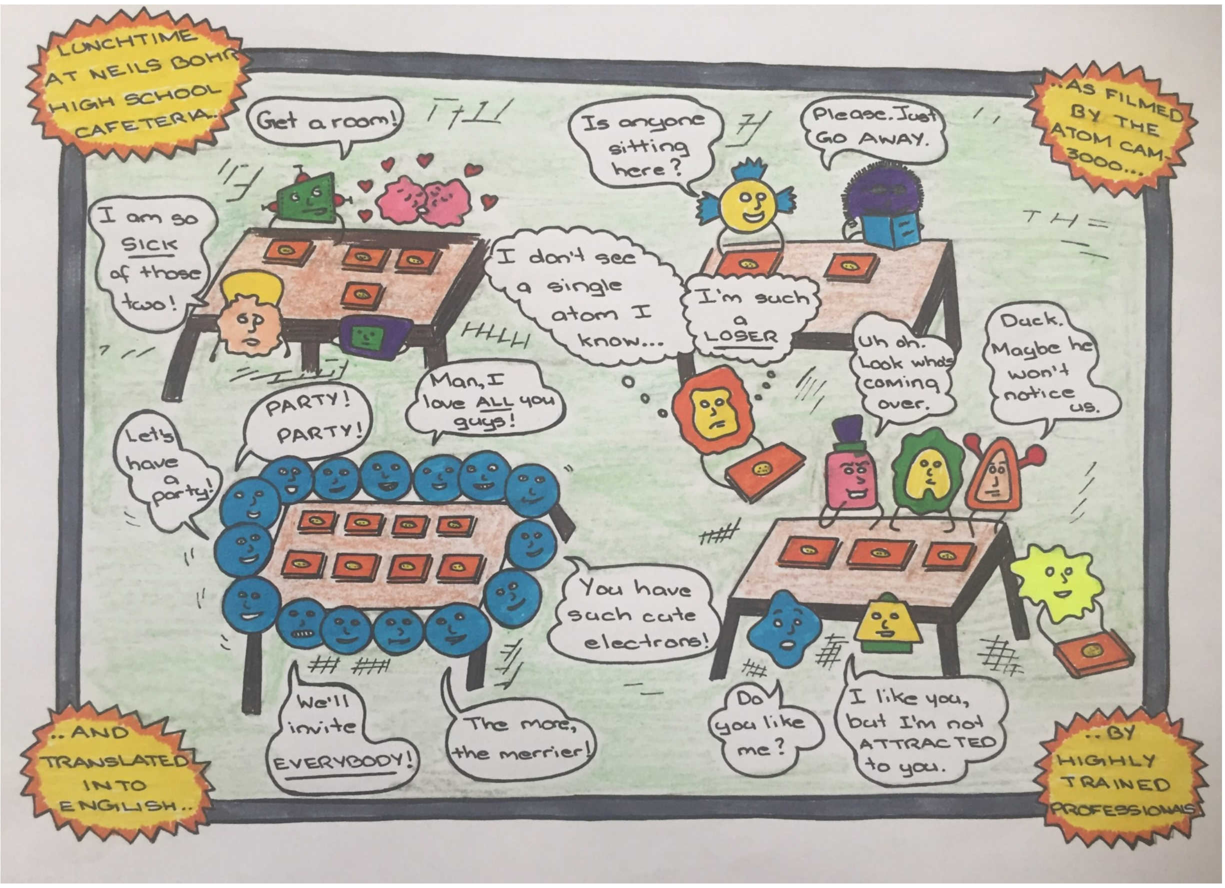
The dire consequences have led to the development, discovery and applications of many ideas and compounds that can be used to lower the effect of the toxin and the formation of rashes and skin eruptions, the simplest solution being, having a bath in cold water. Certain compounds like $Zn(CH_3COOH)_2$, $ZnCO_3$, ZnO , calamine , Burrows Solution (Aluminium Acetate) etc. have been mixed up and used at different doses depending on the severity of the reaction. Non Prescription Oral ***diphenylhydramine (Benadryl)*** is also used. In some cases, *triamcinolone* or *prednisone* is also used. = Benadryl

It has been seen in the latest of the two studies, that the increasing air pollution which contributes manifold for the rise in carbon dioxide levels in the atmosphere, is responsible for the development of stronger and bigger Poison Ivy plants. These larger plants produce a much more potent and plentiful ***Urushiol***, which is obviously more difficult to treat.

Homoeopathic medicines benefice the Ivy by literally putting it to good use. ***Rhustoxicodendron***, commonly known to us as ***RhusTox,*** is widely used therepautically in two main regions of human complexities, skin abnormalities and musculoskeletal injuries.

ARINDAM PAL, 1 BCZ





JASMIN THOMAS 1 M.Sc

MOLECULAR DREAMS

For ages, we have been striving to isolate the different fields of Science as distinct units, perhaps due to misconceptions or some misdirected competitive spirit against those who have taken up a different specialization than you. Physicists won't stop arguing that everything in the universe is just an outcome of some interactions at the microscopic or macroscopic level according to the physical laws which seem to govern them. Mathematicians would counter this by stating that all these laws emerge as a result of abstract mathematical structures, relations and symmetries (or asymmetries). Chemists would mirror them as well. You might be more fascinated by one subject and possibly wish to pursue it further, but there is no logic in being repelled from the other fields in the process. Specialists from any of these fields can convince you that working in that field can be fun; but it is my intention to showcase their implicit unity.

This field originated as a dream, a vision to realize something beyond any practical imagination. It was initially treated in the exact manner as any impractical idea usually is, with incessant criticism and blind ignorance. This field serves as the *ultimatum* for device miniaturization.

Imagine molecular gears that oscillate against each other as they are stimulated by the addition or removal of a single electron, or a domino like arrangement of molecules in which a small perturbation on one end initiates a molecular-mechanical cascade that ripples through the whole assembly in a predetermined fashion. Imagine a wire in which the presence or absence of a single atom dominates the electrical conductivity, or in which a biomolecular recognition process is used to open up new conductivity pathways. These descriptions are respectively those of a molecular-mechanical switch that forms the basis of a random access memory circuit, a molecular-based three-input mechanical Boolean sorter, a single-molecule electrically or magnetically gated switch, and a single-stranded DNA wire that is "turned on" by hybridization of the DNA into the double-stranded form. These molecular systems, and a host of other equally diverse chemical species, are principal actors in the rapidly emerging field of **molecular electronics**. Molecular Electronics can be understood as the field wherein systems consisting of a single molecule (or perhaps few molecules) are investigated and attempted to be realized which could mimic the role of electronic components like diodes, transistors, memory bits on CDs, photovoltaic cells or LEDs.

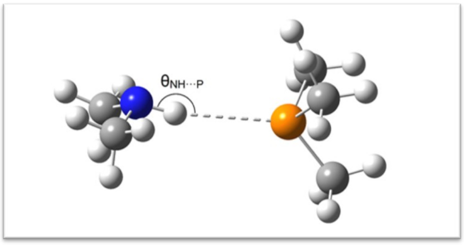
In spite of my motive to demonstrate an inherently unified nature, for conventional reasons, I must state that the synthesis of such molecules (generally organic) is foremost a chemistry problem. Taking a simple case to understand the problem, a molecule destined to be used as a switch must contain three essential terminals – the source, the drain and the gate – when an appropriate signal is applied to the gate, current runs across the molecule towards the drain and when this signal is withdrawn, no charges must flow. This is the simplest application of a transistor, millions of which are found inside each computer component at any time whether it is the CPU, monitor or keyboard.

The imminent challenges that must be faced are – phenomenon of **charge transport** across the electrode to the molecule and through it, the **stability** of the organic molecules to wide range of environmental conditions, **asymmetric** synthesis, **reproducibility** of nanostructures, **density of desirable molecular states** of excitation**, band gap engineering**, better techniques of **fabrication, characterization and measurement of properties** which also allow us to **manipulate** the basic structure to improve the net output, thus efficiency. The important inventions of super-resolved spectroscopies and scanning probe microscopies have contributed abundantly to this field, though we still continue the search for better ways of modifying the material to extract the desirable properties.

I humbly urge you to foster a strong sense of subjective harmony between these seemingly separate fields including biology and any other science you can think of, and utilize your knowledge from one field to evolve novel and creative innovations in another to expand the horizons of human capabilities and venture beyond the unknown.

IR SPECTROSCOPY STRETCHES KNOWLEDGE OF HYDROGEN BONDING

Scientists in Denmark have, for the first time, detected a hydrogen bond between an N–H and phosphorus in the gas phase.



The researchers have detected and N–H···P bond in gaseous dimethylamine–trimethylphosphine complex © American Chemical Society

Hydrogen bonding has been extensively studied in recent years as scientists have attempted to visualise it, with debatable success. But there are still a variety of hydrogen bond acceptors that have yet to be detected, as spectroscopic techniques are not sensitive enough to analyse faint traces of these elusive molecular linkages. Many common bond donors, such as F–H, O–H and N–H, have been identified, but phosphorus as an acceptor has been difficult to pin down as it is widely regarded as a very weak hydrogen bond partner.

The team at the University of Copenhagen has now successfully identified this acceptor in an N–H···P form within a gaseous dimethylamine–trimethylphosphine complex. Using Fourier transform infrared spectroscopy, they searched for any redshifts brought about by the periodic stretching of N–H bonds – a typical sign of any external influence from a bond acceptor. Henrik Kjærgaard and colleagues established that, in this environment, phosphorus has a similar acceptor bond strength to sulfur and is markedly stronger than an oxygen acceptor.

KEZIA SASITHARAN, 1M.Sc

'SUPERBALLS' CAN BLOCK INFECTION BY EBOLA VIRUS !!

Molecular 'superballs' have been created that can stop viruses infecting cells. The molecules, which are based on C_{60} fullerenes, are water soluble and biocompatible, and have shown promise invitro in preventing infection of cells by the Ebola virus.

The dendrimeric 'superballs' bind to glycoprotein receptors where they inhibit viral infections © Courtesy of Jean-François Nierengarten

Animals' immune systems can be alerted to an attack by a virus when it binds glycoprotein receptors on the surface of some cells. This can provoke an immune reaction and prevent infection. However, certain viruses such as HIV and Ebola bind to the receptor and use it as a way to infiltrate the cell, circumventing the immune system.

It is possible to prevent the virus from slipping into a cell by filling the receptor with another molecule with greater affinity. Branched molecules, known as dendrimers, with sugars at the end of each branch have been used in the lab to bind to target receptors. However, large dendrimer synthesis is complex. Now a new type of molecule, using a three-dimensional carbon nanostructure as a scaffold, has been synthesised.

The 'superballs' are macromolecules composed of a core C_{60} fullerene unit, attached to a series of long chain molecules. At the end of each chain is another fullerene, with a shell of mannose carbohydrate units. The globular shape of these molecules mimic the shape of many types of virus, giving a good fit to the receptors. The molecules can be constructed in one pot using copper 'click' reactions, which reduces reaction time and gives excellent atom efficiency. The nature of the reaction means that it is simple to substitute different sugars or biomolecules on the surface, allowing the superballs to be modified for many applications. Tests invitro showed that the superballs were potent inhibitors of Ebola infection in sub-nanomolar concentrations.

KEZIA SASITHARAN 1 MSc

Chemical compounds with weird and astonishing names

Chemistry is a wonderful subject but so is English. Few usual reactions are bound to happen when Chemistry and English come together. Names of the following compounds are result of such weird reactions between the two subjects.

Christite

It is a rare mineral with formula $TlHgAsS_3$ with a bright blood red colour. It is named after the American mineralogist Dr. Charles L. Christ (march on christite march on).

DAMN

Di amino maleonitrile, a cyano carbon that contains two amine groups and two nitrile groups bound to an ethylene backbone.

Constipatic acid

[2-(14-hydroxypentadecyl)-4-methyl-5-oxo-2,5-dihydrofuran-3-carboxylic acid], an aliphatic acid derived from the Australian Xanthoparmelia lichen.

DEADCAT

An apt acronym, given that diethyl azo dicarboxylate is an explosive; shock sensitive; carcinogenic; and an eye, skin, and respiratory irritant.

Draculin

An anticoagulant found in the saliva of vampire bats.

Diabolic Acid

A series of long-chain dicarboxylic acids with chains of different lengths. Named after the Greek word diabollo meaning to mislead.

PEPPSI

PEPPSI is short for Pyridine-Enhanced Precatalyst Preparation Stabilization and Initiation.

Complicatic acid

A sesquiterpenoid antibiotic derived from Stereum complicatum, this is also known as dehydrohirsutic acid.

Moronic Acid

[3-oxoolean-18-en-28-oic acid], a natural triterpene.

Piranha solution

A strongly oxidizing mixture of hydrogen peroxide and sulfuric acid used to remove organic residues from substrates and glassware. The name refers to the voracious appetite of the Amazonian piranha fish.

Sonic Hedgehog

A protein named after Sonic the Hedgehog.

Penguinone

3,4,4,5-tetramethylcyclohexa-2,5-dienone; a two-dimensional representation of its structure resembles a penguin.

Vomicine

Its proper name is deoxynivalenol, but was given the trivial name vomitoxin because it caused vomiting in pigs that had eaten contaminated wheat. It must be pretty gross to make even a pig vomit.

DUMP

Maybe dUMP is the molecule into which all the waste atoms are thrown? In fact dUMP is the acronym for 2'-deoxyuridine-5'-monophosphate, and is an RNA transcription subunit - or a bit of the thing that makes proteins, and is one of the building blocks of DNA.

Pikachurin

A retinal protein named after Pokémon character / species Pikachu. This name was inspired by the parallel between the protein action ("dystroglycan-interacting protein which has an essential role in the precise interactions between the photoreceptor ribbon synapse and the bipolar dendrites", i.e. it enhances visual acuity), and Pikachu's "lightning-fast moves and shocking electric effects".

BABE

This molecule wasn't named for its good looks, or for its resemblance to a film pig. It's actually an acronym of bromo-acetylamidobenzyl-EDTA. BABE is a chelating agent that can be used to bind to proteins, labeling them for subsequent separation and diagnosis.

Frustrated Lewis pairs

As you may know, a Lewis acid is a molecule that bonds to another by accepting a pair of donated electrons, while a Lewis base is a molecule that donates a pair of electrons to form a bond. If there are large, bulky side groups near the donating atom, the donation and/or acceptance of the electrons can be prevented or hindered, and in this case we get what is called 'frustrated' Lewis acids and bases'.

DARSHIKA 1 BCZ