INDIAN INSTITUTE OF TECHNOLOGY PATNA

THC TRIBUNE

(A MAGAZINE FOR CHEMISTRY COMMUNITY)

ON BEHALF OF THRESHOLD CLUB

DIVYANSHU KHANDELWAL

CONTENTS

ALL AROUND THE WORLD

Mysteries of enzymes mechanism revealed

An international research team led by the University of Leicester has made a breakthrough advance by trapping an intermediate in the mechanism of enzymes called heme peroxidases and determining its structure using a beam of neutrons from the heart of a nuclear reactor. The advance is announced in an online publication in Nature Communications.

Link: https://www.sciencedaily.com/releases/2016/11/161129084225.htm

Hydrogen in your pocket? New plastic for carrying and storing hydrogen

A Waseda University (Tokyo) research group has developed a polymer which can store hydrogen in a light, compact and flexible sheet, and is safe to touch even when filled with hydrogen gas. Ketone (fluorenone) polymer can fix hydrogen via simple electrolytic hydrogenation in water at room temperature and release hydrogen when heated to 80 degrees C.

LINK: https://www.sciencedaily.com/releases/2016/11/161128131524.htm

Making graphene using laser-induced phase separation

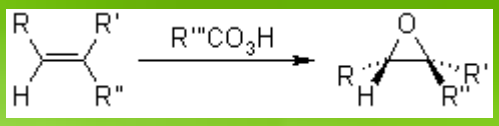
All our smart phones have shiny flat AMOLED displays. Behind each single pixel of these displays hide at least two silicon transistors which were mass-manufactured using laser annealing technologies. While the traditional methods to make them uses temperatures above 1,000°C, the laser technique reaches the same results at low temperatures even on plastic substrates (melting temperature below 300°C). Interestingly, a similar procedure can be used to generate crystals of graphene.

LINK: https://www.sciencedaily.com/releases/2016/12/161201114634.htm

Learning zone

REACTION YOU MUST KNOW

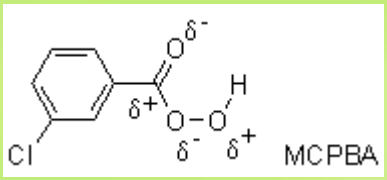
Prilezhaev Reaction



The epoxidation of an alkene with peracid to give an oxirane. The commercial available mCPBA is a widely used reagent for this conversion, while magnesium mono-perphthalate and peracetic acid are also employed.

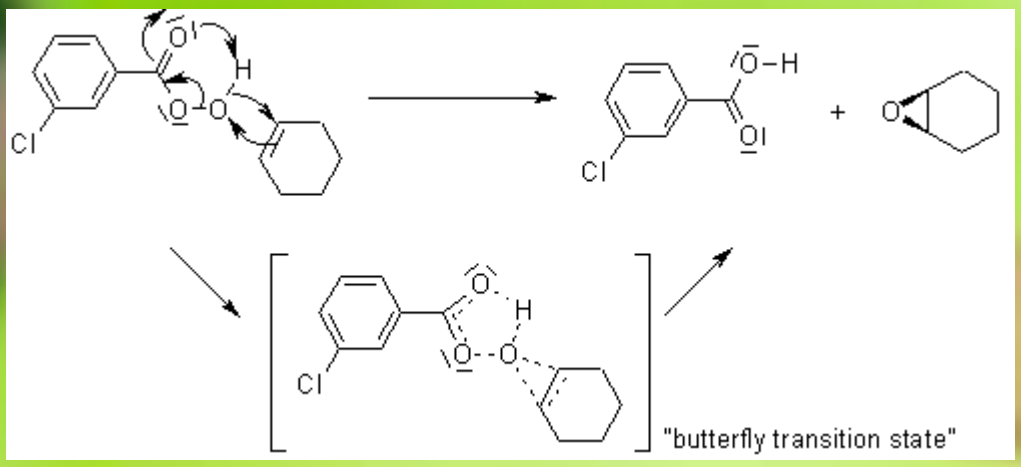
Mechanism of the Prilezhaev Reaction

Peracids tend to adopt an intramolecularly hydrogen-bonded conformation in solution, and the high degree of polarisation results in an electrophilic oxygen atom that is able to add to alkenes.



Hydrogen peroxide in combination with various additional catalysts may also be used in these epoxidations .

The transition state, in which oxygen is added and the proton is shifted simultaneously, resembles a butterfly and is known as the "Butterfly Mechanism":



INFORMATION ZONE

BHABHA ATOMIC RESEARCH CENTRE (B.A.R.C)

The **Bhabha Atomic Research Centre** (**BARC**) is India's premier nuclear research facility based in Trombay, Mumbai, Maharashtra. BARC is a multi-disciplinary research centre with extensive infrastructure for advanced research and development covering the entire spectrum of nuclear science, engineering and related areas.

BARC's core mandate is to sustain peaceful applications of nuclear energy, primarily for power generation. It manages all facets of nuclear power generation, from theoretical design of reactors, computerised modelling and simulation, risk analysis, development and testing of new reactor fuel materials, etc. It also conducts research in spent fuel processing, and safe disposal of nuclear waste. Its other research focus areas are applications for isotopes in industries, medicine, agriculture, etc. BARC operates a number of research reactors across the country.

ELIGIBILITY:

For Engineering Disciplines

B.E. / B.Tech. /B.Sc. (Engineering) with a minimum of 60%* aggregate marks in any of the following engineering disciplines

Mechanical Engineering, Chemical Engineering, Computer Engineering, Electrical Engineering, Metallurgical Engineering, Instrumentation Engineering, Civil Engineering, Electronics Engineering (Related degree disciplines such as Electronics & Communication, Electronics and Controls, etc are also admissible)

Applicants opting to be considered on the basis of GATE Score should have valid GATE Score in the same engineering discipline as the qualifying degree discipline.

Those having qualifying degree in branches like Aerospace, Automobile, Industrial Production, Reliability, Ceramics, Architecture, Geology, Mining, Bio-Medical Electronics/ Instruments, Communication, Information Technology, Master of Computer applications, Dyes & Dye Intermediates, Electrochemical, Energy Systems, Oils & Fats, Paints & Varnishes, Petrochemicals, Plastics, Paper, Sugar Technology, Textiles, etc, are **not eligible**.

Age Limit

- General Category - 26 years
- OBC-29 years
- SC/ST–31 years
- Dependents of those who died in the riots of 1984 (Dep1984) -31 years
- Persons domiciled in Kashmir division of Jammu and Kashmir State from 01/01/1980 to 31/12/1989 (DomKashmir) – 31 years.
- Physically Challenged persons are eligible for age relaxation of maximum up to 10 years.

FUN ZONE

CHEMISTRY WORDSEARCH

Famous Chemists

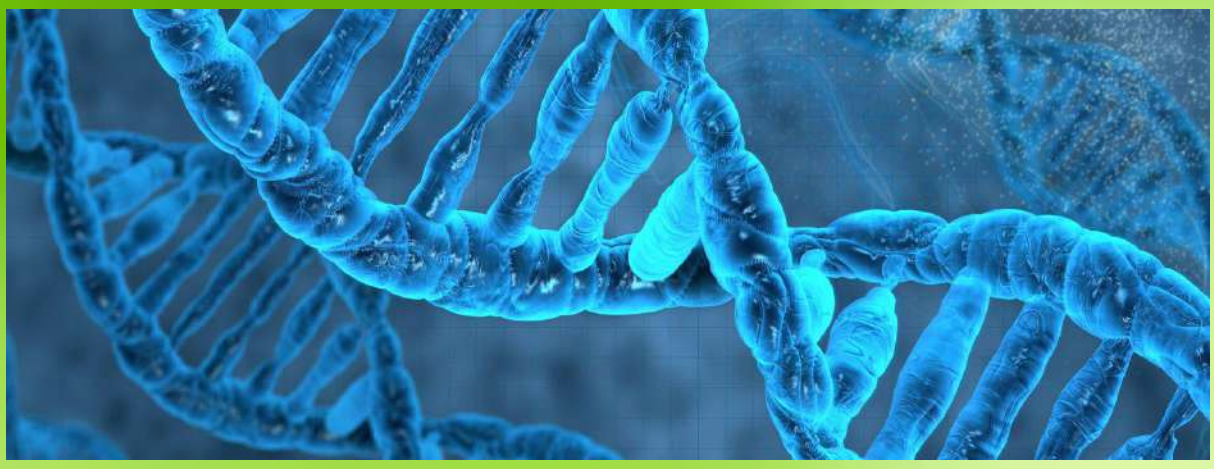
C C L M N M W G Z I R G R O G L U D L O
A K U I R E R S R P A N U E E L S D P M
T S E R E N R U E N K L A P R O T H D A
S I U E I D H N P R E L E W I S C E M T
L O E I U E A H S R E W M I U C R V E T
B T L R N L O O L T I I L I M H O O H B
H R E I L E L T A H C E L A G M O E H N
O U E L A E H P A R K E S I N I K D E S
L O H I Y V N R W V Z E B T A D E E B O
R C C I S O T M R R O B U S L T S E E N
P N S A N I B U E A S G U V S Y R R N A
R A M S A Y O B D Y R S A N I K R E P M
E H U I B H A V N I E W O D S R S N T L
A C T L B W Y V A D D R O F R E H T U R
L I T R I I U B V L B R K B A O N I U O
L N E O B N E R N I L E S B P O O E P N
L O O A H U G A I L E B O N P P T M E Y
B R L A T R B R E S G R D U H S L O N S
U S H O E U L S I E G N D O A I A S E R
N N W H R C I I R R O O Y P U T D R C E

ARRHENIUS
AVOGADRO
BERZELIUS
BOYLE
BRONSTED
BUNSEN
CHANCOURTOIS
CROOKES
CURIE
DALTON
DAVY
DOW
DUPONT
ERLENMEYER
GIBBS
HAHN
KLAPROTH
KREBS
LANGMUIR
LAVOISIER
LE CHATLELIER
LEWIS
LOSCHMIDT
MEITNER
MENDELEEV
NERNST
NEWLANDS
NOBEL
PARKES
PASTEUR
PAULING
PERKIN
PRIESTLY
RAMSAY
RUTHERFORD
SCHEELE
SEABORG
SODDY
VAN DER WAALS

NOTE: Words can be from upward to downward(vice-versa), left to right(vice-versa) and diagonally.

EXPLORE ZONE

BIOCHEMISTRY



Biochemistry, sometimes called biological chemistry, is the study of chemical processes within and relating to living organisms. By controlling information flow through biochemical signaling and the flow of chemical energy through metabolism, biochemical processes give rise to the complexity of life. Over the last decades of the 20th century, biochemistry has become so successful at explaining living processes that now almost all areas of the life sciences from botany to medicine to genetics are engaged in biochemical research. Today, the main focus of pure biochemistry is on understanding how biological molecules give rise to the processes that occur within living cells, which in turn relates greatly to the study and understanding of tissues, organs, and whole organisms—that is, all of biology.

Biochemistry is closely related to molecular biology, the study of the molecular mechanisms by which genetic information encoded in DNA is able to result in the processes of life. Depending on the exact definition of the terms used, molecular biology can be thought of as a branch of biochemistry, or biochemistry as a tool with which to investigate and study molecular biology.

CHEMISTRY IN EVERYDAY LIFE

The secret about smog

On a cold winter morning, if you take a walk outside in our nation's capital, you are likely to be surrounded by a thick cloud of smoke. And you may not be able to see anything at all. This is because of smog. Here is a little clarity about why things get smoky during the winters.

Particulate matter!

Smog forms when sunlight reacts with nitrogen oxides and volatile organic compounds in the atmosphere. These result in tiny particles forming in the air called particulate matter, and ground level ozone.

Smog is made up of unhealthy substances called pollutants. These include smoke from automobiles, fine particles from factories and construction sites. The most harmful pollutants are ground level ozone and small particulate matter. Smog is not the magical misty cloud that you see in movies; it's a harmful cloud of smoke. Smog can make your eyes itchy, give you a sore throat and make it hard for you to breathe. Smog can even make it difficult for your body to fight against infection.

Where smog occurs?

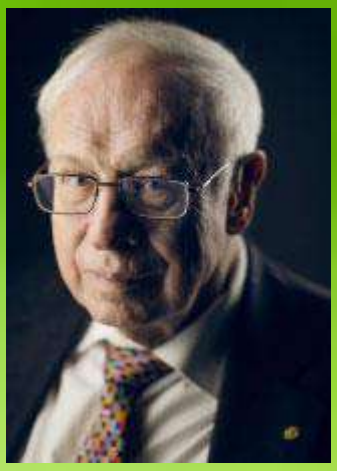
Smog can occur in any place where there is lot of pollution. It is mostly in places surrounded by hills and mountains.Places that have warm, sunny weather can have smog as the warm air prevents vertical air circulation. If there is no wind, pollution cannot blow the smog away to another place. It remains still.

What you can do to prevent smog?

Now that you know how harmful smog can be; it's time to do your bit to stop smog. Since one reason for smog is automobiles, try to avoid using them unnecessarily. When travelling short distances, either walk or use a bicycle. Use public transport when you have to travel long distances.

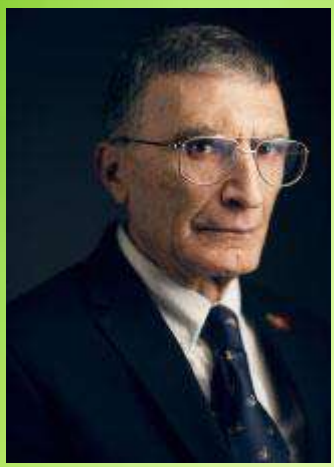
NOBEL LAUREATES IN CHEMISTRY

Tomas Lindahl, Paul Modrich and Aziz Sancar (2015)



Tomas Lindahl

Paul Modrich



Aziz Sancar

The Royal Swedish Academy of Sciences has decided to award the Nobel Prize in Chemistry for 2015 to **Tomas Lindahl** (Francis Crick Institute and Clare Hall Laboratory, Hertfordshire, UK) ,**Paul Modrich** (Howard Hughes Medical Institute and Duke University School of Medicine, Durham, NC, USA) and **Aziz Sancar** (University of North Carolina, Chapel Hill, NC, USA) *"for mechanistic studies of DNA repair"*

The cells' toolbox for DNA repair

The Nobel Prize in Chemistry 2015 is awarded to Tomas Lindahl, Paul Modrich and Aziz Sancar for having mapped, at a molecular level, how cells repair damaged DNA and safeguard the genetic information. Their work has provided fundamental knowledge of how a living cell functions and is, for instance, used for the development of new cancer treatments.

Each day our DNA is damaged by UV radiation, free radicals and other carcinogenic substances, but even without such external attacks, a DNA molecule is inherently unstable. Thousands of spontaneous changes to a cell's genome occur on a daily basis.

The reason our genetic material does not disintegrate into complete chemical chaos is that a host of molecular systems continuously monitor and repair DNA. The Nobel Prize in Chemistry 2015 awards three pioneering scientists who have mapped how several of these repair systems function at a detailed molecular level.

In the early 1970s, scientists believed that DNA was an extremely stable molecule, but Tomas Lindahl demonstrated that DNA decays at a rate that ought to have made the development of life on Earth impossible. This insight led him to discover a molecular machinery, *base excision repair*, which constantly counteracts the collapse of our DNA.

Aziz Sancar has mapped *nucleotide excision repair*, the mechanism that cells use to repair UV damage to DNA. People born with defects in this repair system will develop skin cancer if they are exposed to sunlight. The cell also utilises nucleotide excision repair to correct defects caused by mutagenic substances, among other things.

Paul Modrich has demonstrated how the cell corrects errors that occur when DNA is replicated during cell division. This mechanism, *mismatch repair*, reduces the error frequency during DNA replication by about a thousandfold. Congenital defects in mismatch repair are known, for example, to cause a hereditary variant of colon cancer.

The Nobel Laureates in Chemistry 2015 have provided fundamental insights into how cells function, knowledge that can be used, for instance, in the development of new cancer treatments.

A quantum dot–MUC1 aptamer conjugate for targeted delivery of protoporphyrin IX and specific photokilling of cancer cells through ROS generation

This is one of the research work of Associate Professor Prolay Das along with the research scholars Seema Singh, Pravin Jha, Vandana Singh, Kislay Sinha and Manoj K. Singh

Abstract

Non-targeted photosensitizers lack selectivity that undermines the potential use of photodynamic therapy (PDT). Herein, we report the DNA mediated assembly of a ZnSe/ZnS quantum dot (QD)-photosensitizer (PS)-Mucin 1(MUC1) aptamer conjugate for targeting the MUC1 cancer biomarker and simultaneous generation of reactive oxygen species (ROS). A photosensitizer, protoporphyrin IX (PpIX), was conjugated to a single stranded DNA and self-assembled to a complementary strand that was conjugated to a QD and harboring a MUC1 aptamer sequence. A multistep fluorescence resonance energy transfer (FRET) is shown that involves the QD, PpIX and covalently linked CF™ 633 amine dye (CF dye) to the MUC1 peptide that tracks the potency of the aptamer to attach itself with the MUC1 peptide. Since the absorption spectra of the CF dye overlap with the emission spectra of PpIX, the former acts as an acceptor to PpIX forming a second FRET pair when the dye labeled MUC1 binds to the aptamer. The binding of the QD-PpIX

nanoassemblies with MUC1 through the aptamer was further confirmed by gel electrophoresis and circular dichroism studies. The selective photodamage of MUC1 expressing HeLa cervical cancer cells through ROS generation in the presence of the QD-PpIX FRET probe upon irradiation is successfully demonstrated.

Conclusion

Herein,we have demonstrated the preparation of nanoassemblies constructed from aqueous soluble ZnSe/ZnS QDs and the PpIX FRET probe conjugated to the MUC1–aptamer. Either of the nanoassemblies, where the QD is directly conjugated to the PpIX or through DNA hybridization, is able to detect cancer cells through the aptamer based recognition of the cancer cell bio-marker MUC1. We evaluated the binding event of these FRET probe–aptamer assemblies to the MUC1 peptide by covalent coupling of the CF dye to the MUC1 peptide. A second FRET event between PpIX and CF dye was observed when QD–PpIX FRET pairs come in contact with the MUC1–CF dye conjugate. The targeted release of ROS through PpIX was also observed following its excitation through QD mediated FRET. Furthermore, the cell viability of RAW (macrophage cells) and HeLa (Humancervical cancer cells) cell lines was evaluated in the presence of these nanoassemblies. The decrease in the cell viability of specifically MUC1 expressing HeLa cells is attributed to the ROS

Quantum Dot-MUC1 Aptamer Conjugate for Targeted Delivery of Protoporphyrin IX and Specific Photokilling of Cancer Cells through ROS Generation. Available from: https://www.researchgate.net/publication/307092690_Quantum_Dot-MUC1_Aptamer_Conjugate_for_Targeted_Delivery_of_Protoporphyrin_IX_and_Specific_Photokilling_of_Cancer_Cells_through_ROS_Generation [accessed Jan 6, 2017].

Q & A ZONE

You all might be reading this expecting that you will get to know about someone's experience of internship. Well of course you will, but today we have with us Ms Apoorva Shrivastava (Btech pre final year student),someone who really can teach us much more than that. Take a look on a chat session she had with us sharing her memorable internship experience .

ThC: Please tell us about the project work you did.

Apoorva: I went there in hopes of learning some computational chemistry dealing with some quantum computations and mathematics but ended up learning Dissipative Particle Dynamics Simulations which is basically a stochastic method to simulate dynamic fluids. Simulations were performed on different surfactant molecules to calculate the Critical Micelle Concentration at different concentrations using several softwares like LAMMPS, VMD and learnt various computational methods.

Well in easy terms I began with an infinite set of papers, books and questions in my head and started with single molecules and then pairs experimenting with softwares and then creating layers and actual systems. The most fascinating part and my motivation were my PhD Labmates, they were all doing incredible works on Ionic liquids, polymers and proteins that could be incredible discoveries in the field of electronics, drug discovery and explanations to the several unknown questions.

You can see more about simulations via Google and get some more terms from this article on future of Molecular simulations here -

http://onlinelibrary.wiley.com/doi/10.1002/aic.690481202/pdf

ThC : How did you manage to get an internship in 2nd year? Tell us about the problems you faced while applying?

Apoorva: Well I was looking for one since my first yr, being from a business family,I want to get in something of my own asap. I wrote a hell lot of mails, from IIT's to IIM's , from HUL to startups. Got a few major replies and chose to go to JNCASR as the Prof is the best in India in his field and I was more

interested into his work then rest of the options considering my future prospects and benefits from this internship. Talking of the problems faced, one applying in the industry must have some contacts out there, it hardly works without that but a considerably good resume with some relative work experience and good CPI might get you a research intern (exceptions are always there :)) I didn't had any contacts in the industry but being a very talkative person and persistency to keep on searching for companies and HRs led me to IOCL, BASF, Tata Chemicals but they were all offering me interns in the field I didn't wanted to work in, so kept them as a backup option. There are many summer and winter intern programs like IAS, JNCASR and many more but I was too late to apply to any of them so writing mails was the only thing I could do, which at the end worked for me. The only problem in my case was I applied very late, I was too scared or unsure to get into core Chemical which really misleaded me for a quite a long time. We are very naive and hitting a topic just like that to work on for a period of 3 months or may be in future as well seems to be a huge thing, but a little push in one direction tells us if it is right or wrong and then all humans are cursed to make mistakes and learn, risk is all we can take if nothing else is available for free.

Though Simulations is not that much of a risk to me but a combination of branch, interest and fascination I should say.

ThC: What are the benefits of doing such internships? Is it really necessary to apply for such internships in 2nd year itself?

Apoorva: Not necessary but surely better than sitting at home idle. Doing some online courses is also good but working with people of similar age and interest in a different city gives you a different exposure and learning. I was accommodated in IISc, went to almost all the labs and was always crowded with scientific heads around me.

ThC: We have also heard about you getting a foreign internship for the upcoming summer. Please tell us about it.

Apoorva: I applied to almost all the top Universities in India as well as outside, and out of a few people who accepted my application and agreed to provide the funds, I chose to go to OHSU, Portland under Prof. Daniel Zuckerman, he was previously at Univ. of Pittsburgh and recently shifted to OHSU for a project by NIKE on parts of which I will be working on.

ThC: Suggestions for juniors!

Apoorva: Internships are no big deal, stay back and work on your own, may be on a project making a prototype or your own start-up, learning is all what matters. Your branch will not decide who you are, you will decide what any branch can be! You can make it with the pointers and without the pointers. It's your own battle we can only advice and share our experiences, no blood will shed till you get your weapons out.

ThC : We are really thankful to you for sparing some time for us from your busy schedule and congratulations for your upcoming internship.