



Computer Aided Drug Designing

By

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XI-B



INTRODUCTION

On 19 August 2019, students of class 10 and the science sections of class 11 and 12 got a chance to dive into the microscopic world of drugs in an interactive session with Dr Indrakant K. Singh, associate professor in the field of Molecular Biology, Biotechnology and Bioinformatics at Deshbandhu College.

INTERACTION

- Dr Singh began his lecture by defining the science of medicine as one of uncertainty and an art of probability.
- Taking us across the Central Dogma of Biology and the Complexity of The Human Genome, he imparted astonishing facts that were beyond belief.
- His explanation of the structure of a protein and its various stages; humorous manner of defining the term 'drug' brought all to attention and saw them engage in a lively discussion on the same.
- Having given all the information about action of drugs on the body, its basic structure, ways of manufacturing drugs and how computer programming helps in deciding most effective structure of drug, Dr Singh conducted a quick Q/A round to recapitulate the salient points of the discussion before speaking on two new topics - Cheminformatics and Bioinformatics.
- A brief brush over inventive and present drug designing techniques, the time and effort spent to get them onto our chemist shops' shelves, the ways adopted to select a disease, ligands, molecular docking and ADMET simulation held the audience spell bound for another half-an-hour.
- The inquisitive children asked questions to clarify whatever doubts they had, and Dr Singh answered all of them with a

smile on his face, happy to see the level of interest the students were taking in the subject.

CONCLUSION

- In the end, Dr Singh talked career opportunities in the field of medicine despite the cut throat competition. He elucidated names of some Gene-Editing-Simulation-Games, and showed videos on “Drugs and Drug Targets”, and also, ACE Inhibitors.
- In his concluding statement, he said that drug designing is a complex process with multidisciplinary aspects which needs collaboration of humans and artificial intelligence for its optimum utilisation.

AMAZING FACTS

Human genome contains 3 billion (300,00,00,000) base pairs.

Each pair has 30,000 unique genes.

There are 10-100 variants of genome through alternate splicing.

Any gene (or, its product) can be a potential drug target.

There are approximately 500 unique targets.

There are 10^{200} potential small molecules.

Given below is the URL of one of the videos shown to the audience.

<https://youtu.be/u49k72rUdyc>