Report on Short Term Certification Course On Computer Aided Drug Design And Molecular Docking Held On 04.04.2022 – 09.04.2022

Date of Event	04.04.2022 – 09.04.2022
Name and Type of Event	Short Term Certification Course On Computer Aided Drug Design And Molecular Docking
Conducted by	**SCHOOL OF PHARMACY, ARKA JAIN University**
No. Of Participant	**30**

A short term certification course on **computer aided drug design and molecular docking** was organized from 4th April 2022 to 9th April 2022 School of Pharmacy, ARKA JAIN University. On this occasion DR. CHITA RANJAN SAHOO, Senior Research Fellow from Indian Council of Medical Research, Govt. of India, and Bhubaneswar) has instructed the students as guest faculty. Dr. Jotirmaya Sahoo, Dean, School of Pharmacy has developed and designed the course. Miss Yogita Kmari, Asst Professor, School of Pharmacy coordinated the program. The objective of the course is, in recent years, bioinformatics has emerged as a critical component of research in the fields of Pharmaceutical, biomedical, and drug discovery. Researchers, faculty, and students interested in learning about cutting-edge bioinformatics methods will all benefit from this workshop. It is designed to curiosity researchers' interest and aid in the improvement of their research methods in advancement of drug design. The course is structured with three modules for six days. Every day there will be 5 hours of classes. The students appeared assignments and assessment to qualify the course. Honourable Vice Chancellor Dr. S.S. Razi, Director Mr. Amit Shrivastav, Registrar Mr. Jasbir Singh Dhanjal and Dean Student Welfare Mr. Angad Tiwari, Head of The Department of CS & IT Mr. Arbind Pandey and CFO Mrs. Richa Garg along with other eminent persons of the University felicitated Dr. Chita Ranjan Sahoo offering with flower bouquet and shawl. On last day a certificate of appreciation presented to Dr. Chita Ranjan Sahoo. Students were awarded with certificates after successful completion of 6 days (30 hours) course.

On completion of course, students learnt many things about computer aided drug design and molecular docking. Drug development is an expensive and cumbersome process. Pharmaceutical companies suffer huge monetary loss due to failures of the lead candidates at the later stages of drug discovery process. For bringing a single drug molecule to the market more than 10,000 compounds are screened. These drug development process accounts for about 156 million USD in the discovery phase and about 75million USD in FDA processes which sums up to approximately 231 million USD. Further, extensive exorbitant procedures are to be followed for gaining FDA approval. Computational approaches are of immense advantage to reduce the chance of later stage failures of the lead candidates, speeds up the molecular screening process and are economical. Computer Aided Drug Design (CADD) utilizes various bioinformatics and chemoinformatics resources including softwares, databases, algorithms, easily deals with large amount of proteomics,

genomics and transcriptomics data, processes it efficiently and provides potential drug candidates. Norfloxacin, Dorzolamide, Zanamivir, Saquinavir and Oxymorphone are few examples of drugs recently developed with CADD. Moreover, molecular docking, pharmacophore modeling, and QSAR are most frequently used CADD methods.

USED SOFTWARE/WEB-SERVER FOR CADD

1. Database generation : PubChem: Open chemistry database , DRUGBANK: Knowledge bases of drugs
2. Chemical descriptors : ChemDraw, ACD/ChemSketch
2. Molecule converter : Open Babel v3.1.1, Translational medicine-Pasilla.health.unm.edu
3. PASS prediction : Way2drug-online
4. Drug-likeness : Molsoft
5. Lipinski Rule : IIT Delhi Supercomputing facility, Molsoft
6. Pharmacokinetics : AdmetSAR, Preadmet
7. Toxicity : Protox
8. Receptor : Protein Data Bank
9. Protein preparation : Biovia Discovery Studio
10. Docking tool : Autodock , CB-Dock
11. Docking visualization : Chimera, LigPlot+

Agenda 1: Welcome by Dr. Jyotirmaya Sahoo, Dean of School of Pharmacy

Discussion: Dr. Jyotirmaya Sahoo, Dean of School of Pharmacy welcome all the members present with the meeting.

Agenda 2: Title of the STCC.

Discussion: Keeping the importance of drug discovery and drug designing in view the title on which the STCC will be conducted was decided as **Computer Aided Drug Designand Molecular Docking**. The course will be of 6 days (30 hours). Curriculum designing will be done by course developer with assignments and assessments. Two Assignment of 25 marks and one assessment of 50 marks. Total 75 marks. Assessment is of 1.5 hour in offline mode.

Agenda 3: Objective of the STCC.

Discussion: Drug discovery and development is an intense, lengthy and an interdisciplinary endeavour. The contribution of computational methodologies has revolutionized the process of drug discovery. It is a powerful tool in the study of the relationship between molecular structure and biological activity and thus essential in the process of rational drug design. Nowadays, world's major pharmaceutical and biotechnological companies use computational design tools. This Computer Aided Drug Design course covers all main computational techniques used in drug discovery and supply a basic level of knowledge in this research field. This technique will provide a unique platform to screen new drug entities. The recent tendency in drug design is to rationally design potent therapeutics with multi-targeting effects, higher efficacies, and fewer side effects, especially in terms of toxicity. Molecular docking is frequently used in the process of computer aided drug design (CADD). It can be applied in different stages of the drug design process in order to: (1) predict the binding mode of already known ligands; (2) identify novel and potent ligands and (3) as a binding affinity predictive tool.

Agenda 4: Scheduling and Permission from Vice Chancellor

Discussion: It is decided to schedule the course from 28th March 2022. Notice need to be circulated among the students and faculty members after the approval of Vice Chancellor of the University. However keeping the University Annual Sports on view if date need to be extended then revised notice need to be issued. An information in this regard to COE of University and Member Secretary of BOS of SOHAS need to be mailed.

Agenda 5: Invitation to Subject Expert

Discussion: Dr. Chitaranjan Sahoo: ICMR-Senior Research Fellow IMS & SUM Hospital Siksha 'O' Anusandhan Deemed to be University Bhubaneswar, Odisha, India has given his verbal consent over pone to instruct the course as Subject Expert. Later a mail of invitation is decided to be sent and confirmation should be record.

Agenda 6: Budget planning

Discussion: A budget is planned and submitted to accounts section of University. It is decided to register the course by the interested candidates by paying an amount of 800.00 rupees. The to and fro expense of the guest faculty, remuneration, certification, stationary *etc* will be borne from this collection.

Agenda 7: Information to students

Discussion: Students and staffs to be informed through their whatsapp group, website notice board to participate the STCC. All participants need to come with their uniform.

Agenda 8: Promotion

Discussion: Posters and brochure need to be designed by University designer Mr. Gourango and circulated as well as need to be uploaded with the website. Photographs will be with geo tag.

Agenda 9: Event report preparation and submission to In-charge Website and official documentation and Press Release

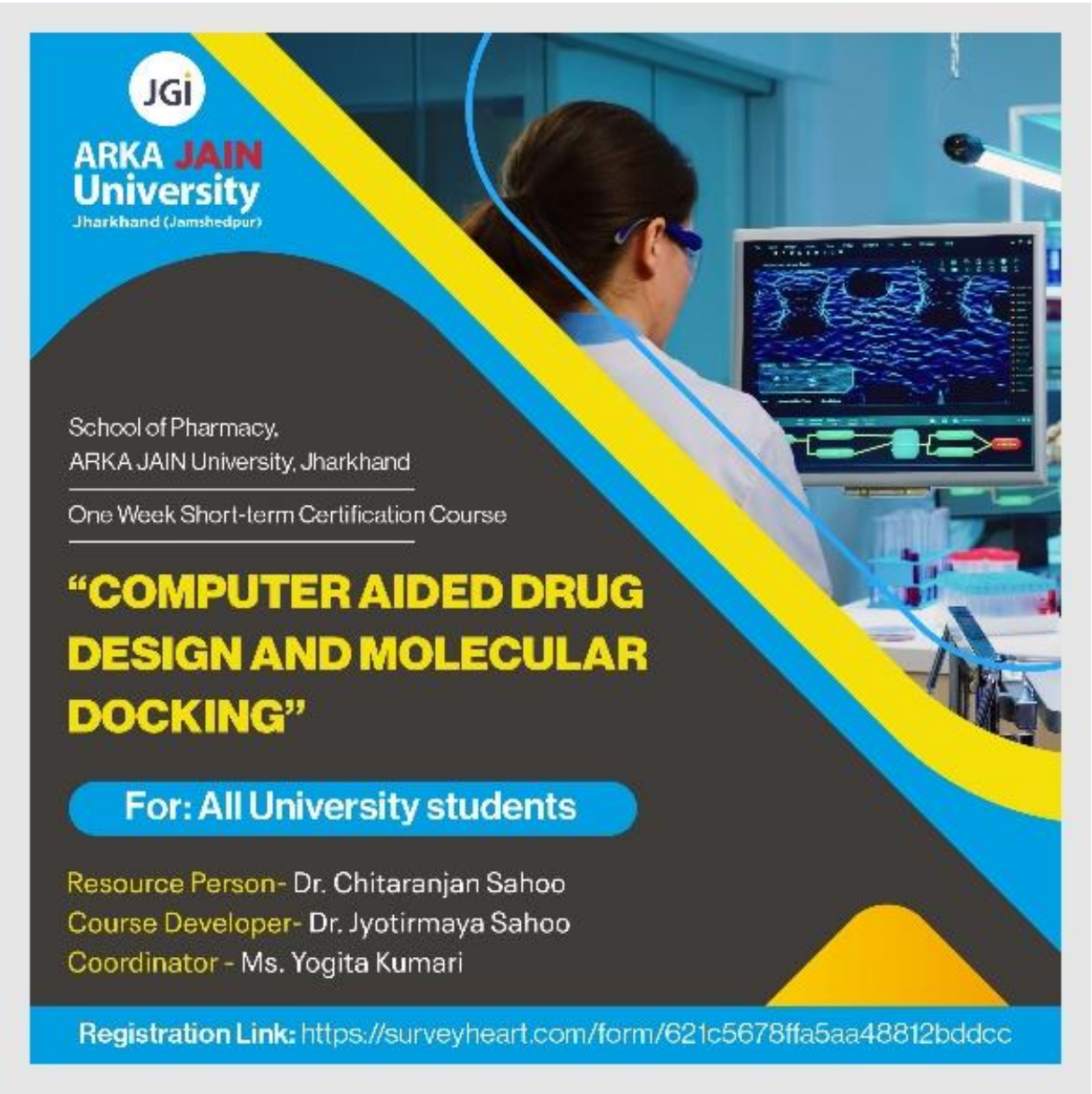
Discussion: Event report to be prepared and submitted to In-charge Website immediate after completion of the event and also need to be submitted with key highlights and monthly NAAC report to IQAC.

Agenda 10: Record the event by the Website update & Press and Media Committee of School of Pharmacy

Discussion: The event report need to be recorded with the School of Pharmacy.

The Meeting for the **Short Term Certification Course** was closed with vote of thanks to the present members.

Poster of the Event



Glimpse of the Event

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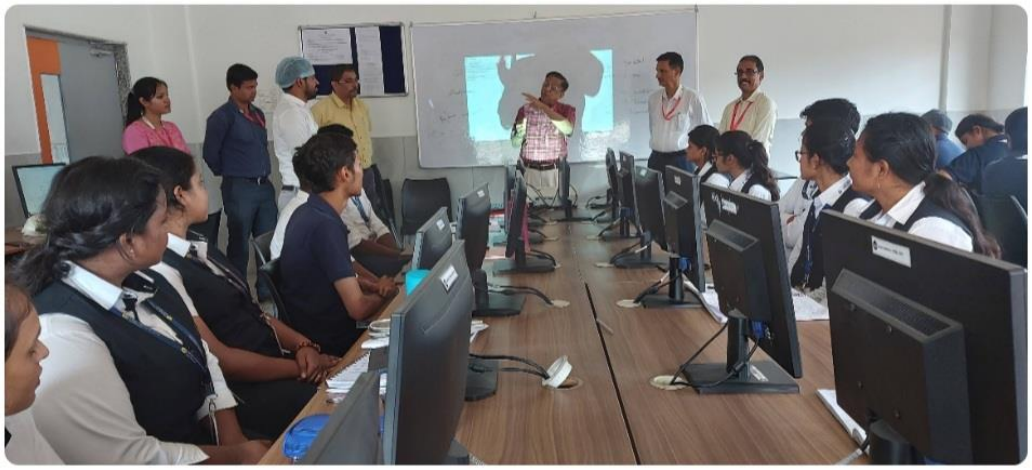
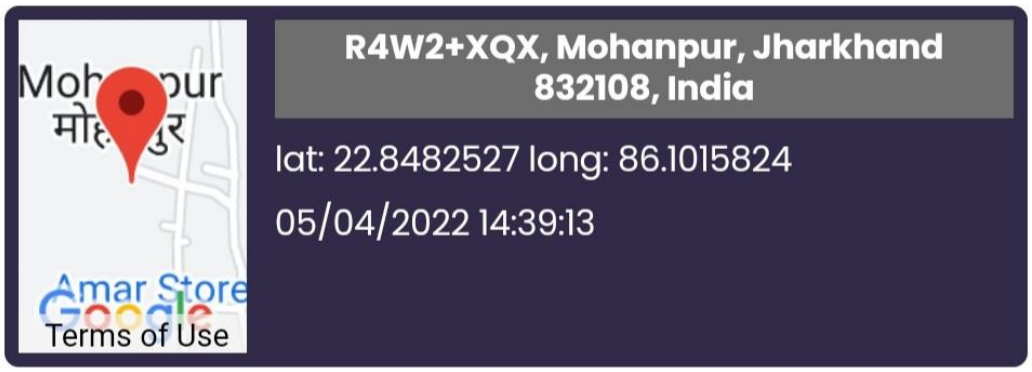
R4V2+3V3, Mohanpur, Jharkhand 832108, India





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