Report On Virtual Screening of Leading Molecules: An In-Silico Approach And Simulated Animal Experiments In Pharmacology Two Days Offline Workshop Held On – 21/09/2021-22/09/2021

Date of Event	21.09.2021-22.09.2021
Student Activity	Virtual Screening Of Leading Molecules: An In-Silico Approach And Simulated Animal Experiments In Pharmacology
Conducted by	School of Pharmacy
No. Of Participant	45

School of Pharmacy, ARKA JAIN University organized "Two days offline workshop" Entitled **"VIRTUAL SCREENING OF LEADING MOLECULES: AN IN-SILICO APPROACH AND SIMULATED ANIMAL EXPERIMENTS IN PHARMACOLOGY".** This workshop was arranged to gain hands-on experience and rapidly acquire knowledge in advanced topics where curriculum-based education is yet to be developed.

Day 1 (21st September, 2021)

The programme commenced with the lighting of the Ceremonial lamp by the Dr S.S Razi (Vice Chancellor), Mr Amit Srivastava (Director), Mr Jasbir Singh Dhanjal (Registrar), Mr Angad Tiwary (Director,Campus), Dr Jyotirmaya Sahoo (Dean, School of health and allied Sciences) and speakers of the workshop Dr. Chitaranjan Sahoo and Dr. Shakti Ketan Prusty followed by Saraswati Vandana. In his brief address to the participants, Honourable Vice Chancellor of AJU, Prof. (Dr) S.S Razi congratulated School of Pharmacy to organising these offline workshops. Welcome address was given by Dean, School of Pharmacy (AJU) Dr. Jyotirmaya Sahoo. The event was hosted by Miss Khusboo Raj, Assistant Professor, School of Pharmacy, ARKA JAIN University.

Welcoming Everyone with Tilak

Session 1: VIRTUAL SCREENING OF LEADING MOLECULES: AN IN-SILICO APPROACH

After Inaugural ceremony session was started after high tea. Speaker of the session 1 was Dr. Chita Ranjan Sahoo. He received PhD at Central Research Laboratory, Institute of Medical Sciences & SUM Hospital, and Department of Pharmaceutical Chemistry, School of Pharmaceutical Sciences, Siksha 'O' Anusandhan (Deemed to be University), Bhubaneswar,

Odisha and former Research Assistant in a National project of TB, funded by National Institute for Research in Tuberculosis at ICMR-RMRC, Bhubaneswar, India and former Junior Research Fellow at Regional Plant Research Centre Bhubaneswar, Odisha. He obtained his Master's degree in Biotechnology, Utkal University, Odisha, India. His doctoral research work, basically on medicinal chemistry approaches to mainstream drug development for UTI-bacteria & breast-cancer. Apart from this, his thrust areas of research interest include; Cyanobacteria, Medical microbiology, nano-synthesis, natural product synthesis and computational chemistry with lead molecule discovery. He is keen in study in details the drug-disease pathway interaction, which presumably aids in the understanding of mechanisms by which several accountable genes and enzyme function related to human cancer. Dr. CR Sahoo has published several peer-reviewed SCOPUS & Science Citation Indexed papers including research articles, review articles, abstracts, book chapter and books with more than 85 impact factors. These are leading houses namely, Wiley, Springer, Springer Nature, Taylor & Francis, Elsevier. Moreover, His contribution towards problem to key solution in research achieving Chief Minister Award- for the year 2016-17 as youth innovation, Young Scientist Award in Science-2018, Rajiv Gandhi Prativa Puraskar Odisha Forum and a few more. By visionary thinking of Dr. CR Sahoo invited as resource person and lecture talk at several organizations. He has been associated with various professional societies, life member association and Odisha divisional coordinator of Green Skill Development program, govt. of India.

Workshop Inauguration with Spiritual Lamp Lighting

The term '*in silico*' is a modern word usually used to mean experimentation performed by computer. *In silico* pharmacology (also known as computational therapeutics, computational pharmacology) is a rapidly growing area that globally covers the development of techniques for using software to capture, analyse and integrate biological and medical data from many diverse sources. More specifically, it defines the use of this information in the creation of computational models or simulations that can be used to make predictions, suggest hypotheses, and ultimately provide discoveries or advances in medicine and therapeutics. It has also been suggested that if we are to build on the advances of the human genome, we need to integrate computational and experimental data, with the aim of initiating *in silico pharmacology* linking all data types. This could change the way the pharmaceutical industry discovers drugs using data to enable simulations; however, there may still be significant gaps in our knowledge beyond genes and proteins.

Honourable Vice Chancellor of AJU felicitating Dr Chita Ranjan Sahoo

Day 2 (22nd September, 2021)

The programme commenced with the lighting of the Ceremonial lamp by the Dr S.S Razi (Vice Chancellor), Mr Amit Srivastava (Director), Mr Jasbir Singh Dhanjal (Registrar), Mr Angad Tiwary (Director,Campus), Dr Jyotirmaya Sahoo (Dean, School of health and allied Sciences) and speakers of the workshop Dr. Chitaranjan Sahoo and Dr. Shakti Ketan Prusty followed by Saraswati Vandana. Speaker of session 2 was Dr. Shakti Ketan Prusty, Assistant Professor, Department of Pharmacology, School of Pharmaceutical Sciences, Siksha O Anusandhan (Deemed to be University), Bhubaneswar, Odisha. He received PhD at School of Pharmaceutical Sciences, Siksha 'O' Anusandhan (Deemed to be University), Bhubaneswar and topic of his research was **Brain delivery of Losartan carboxylic acid and evaluation of its efficacy against stress induced neurodegeneration.** Previously, he worked as Junior Research Fellow, Drug Development and Analysis Lab, School of Pharmaceutical Sciences, Siksha O Anusandhan (Deemed to be University), Bhubaneswar, Odisha. He actively involved in synthetic product development (Project funded by DRDO, LSRB, Govt. of India, New Delhi), Development of analytical methods for new Drug,

Screening of drug activity against various neuro-pharmacological models, Enhancement of brain delivery of new drug. He also expertised in Screening of various drugs in animal models like CNS Drugs, anti-diabetics etc., Animal handling and preclinical studies, Pharmacokinetic studies, Analytical method development for various drugs by HPLC He started his session by briefing the participant about use of animals in research and education and alternative of animal experiments.

Dean School of Pharmacy is Addressing the Gathering

Session 2: SIMULATED ANIMAL EXPERIMENTS IN PHARMACOLOGY

He discussed about use of animals in research and education dates back to the period when humans started to look for ways to prevent and cure ailments. Most of present day's drug discoveries were possible because of the use of animals in research. The dilemma to continue animal experiments in education and research continues with varied and confusing guidelines. However, the animal use and their handling vary in each laboratory and educational institution. It has been reported that the animals are being subjected to painful procedures in education and training unnecessarily. The extensive use of animals in toxicity studies and testing dermatological preparations has raised concerns about the ways animals are sacrificed for these “irrelevant experiments”. On the other side of the coin are scientists who advocate the relevant and judicious use of animals in research so that new discoveries can continue. Thousands of animals are used annually in educational institutes despite efforts by concerned teachers and activists to reduce this number. Many medical schools in India and other countries have either introduced alternatives to these experiments or are deliberating on this contentious issue.

Dr. Shakti K. Prusty and Dr. Chita R. Sahoo Instructed the Workshop

There is a belief that just as medicine cannot be taught or learnt without exposure to wards and clinics, pharmacology cannot be taught without experimentation in animals. However, with changing trends in teaching methods and practices, it is increasingly felt that animals should not be sacrificed just to acquire skills and techniques of experimentation. These experiments are expensive, time consuming and tedious. Also, the availability of animals is becoming sparse. Guidelines by Committee for the Purpose of Control and Supervision of Experiments on Animals (CPCSEA), University Grants Commission (UGC) and the Medical Council of India (MCI), suggest 3 Rs i.e., replacement, refinement and reduction in animal experiments, with the fourth R added, that is their rehabilitation, as an added measure for their care. In this changing scenario, development of alternatives are the need of the day.

Dr. Chita R. Sahoo is receiving the Token of Appreciation from Honourable Registrar of AJU

The use of live animal experiments is decreasing in many medical colleges across India. These are gradually being replaced by certain alternatives that are available at relatively low cost and with proven educational efficacy. In this review, we discuss the evolution of the use of animals in education and research and how these have been affected in recent times owing to concerns from animal lovers and government regulations. He also discussed certain viable alternatives to animal experiments.

A Token of Appreciation is offered by Honourable Registrar of AJU to Dr. Shakti K. Prusty

Alternatives are needed at all stages i.e., initial, interim and final *in vivo* testing. A few examples of these alternatives are:

i. *In vitro* techniques

- Organ cultures
- Tissue slices
- Primary cell cultures
- Established cell lines
- Stem cells.

ii. In Silico (Computer based)

iii. Invertebrate animals Invertebrates can be used to replace the more commonly used laboratory animals. The most used invertebrate species are *Drosophila melanogaster*, a fruit fly and *Caenorhabditis elegans*, a nematode worm. *Drosophila melonogaster* is a classic model used for detecting mutagenicity, teratogenicity and reproductive toxicity. The body of *C. elegans* is completely transparent. Further, the precise lineage of all the organism's cells can be

studied. These organisms have short life cycle and can be studied in large numbers, a distinct advantage over the vertebrates.

iv. Rapid developing vertebrates

A recent vertebrate model, the Zebra fish has proven to a very good model for toxicity testing. Studies on various chemicals have shown that Zebra fish have shown that 90% of these produced specific tissue, organ and behavioral toxicity. These have been used and validated in large scale high throughput screens for various psychotropic drugs.

There were hands on training of ExPharm Software for the participants followed by valedictory program. Both the speakers were felicitated by Dignitaries of ARKA JAIN University. Dean, School of Pharmacy (AJU) Dr. Jyotirmaya Sahoo while delivering a speech on this occasion, said that it was not the events but the attitude that caused success. At the end of programme, Mr. Sumanta Sen, Associate Professor, School of Pharmacy, ARKA JAIN University has delivered vote of thanks to audience.

Successful Ending of Two Days Workshop Witnessed by the Students and Particpants

PRESS RELEASE

अरका जैन यूनिवर्सिटी. स्कूल ऑफ फार्मेसी की दो दिवसीय कार्यशाला में बोले वक्ता

नयी टेक्नोलॉजी और सॉफ्टवेयर के जरिये नये मोलेक्युल्स की खोज संभव

लाइफ रिपोर्टर@जमशेदपुर

अरका जैन यूनिवर्सिटी के स्कूल ऑफ फार्मेसी की ओर से वर्चुअल 'स्क्रीनिंग ऑफ लीडिंग मोलेक्युल्स एन इन-सिलिको एप्रोच एंड सिमुलेटेड एनिमल एक्सपेरिमेंट्स इन फर्माकोलॉजी' विषय पर दो दिवसीय कार्यशाला का आयोजन किया गया. इसमें फार्मेसी के विद्यार्थियों को नये मोलेक्युल्स की खोज में सॉफ्टवेयर के प्रयोग एवं अन्य लेटेस्ट टेक्नोलॉजी की जानकारी दी गयी. शिक्षा एवं अनुसंधान विश्वविद्यालय भुवनेश्वर के डॉ चितरंजन साहू एवं डॉ शक्ति केतन वक्ता व विशेषज्ञ के रूप में

मौजूद थे. डॉ चित्तरंजन साहू ने केमड्रा सॉफ्टवेयर के बारे में विस्तार से चर्चा की. उन्होंने केमिकल स्ट्रक्चर, रिएक्शन एवं जीव वैज्ञानिक वस्तुओं के थ्री-डी स्वरूप देखने का तरीका भी बताया. कहा कि नयी तकनीकों के सहारे हम मोलेक्युल्स की खोज कर सकते हैं. उद्घाटन सत्र को संबोधित करते हुए कुलपति प्रो (डॉ) एसएस रजी ने कहा कि फार्मेसी भारत में एक उभरता हुआ एकेडमिक क्षेत्र है, जहां शोध के कई अवसर हैं.

कुलसचिव जसबीर सिंह धंजल ने प्रतिभागियों से कार्यशाला का लाभ उठाने का आह्वान किया. स्कूल ऑफ हेल्थ एंड अलाइड साइंस के डीन डॉ ज्योतिर्मय साहू ने स्वागत भाषण दिया. अंत में कैंपस डायरेक्टर डॉ अंगद तिवारी ने अतिथियों को सम्मानित किया. संचालन व धन्यवाद ज्ञापन असिस्टेंट प्रोफेसर खुशबू राज ने किया.

प्रभात खबर
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THANK YOU