


विज्ञान एवं प्रौद्योगिकी विभाग DEPARTMENT OF SCIENCE & TECHNOLOGY





Report on

DST STUTI ICT

A hands-on Training Program on Approaches for Screening and **Characterization of Pre-clinical Drug Candidates**

(Dec 8-14, 2022)

Under the Scheme

Synergistic Training Program Utilizing the Scientific and Technological Infrastructure

(STUTI)

An Initiative by

The Department of Science and Technology, India

Organized by The Institute of Chemical Technology, Mumbai (PMU)

Organized by

Department of Biotechnology and Bioinformatics, JUIT



Hosted by Jaypee University of Information Technology (JUIT) Waknaghat, Solan

Report on Seven Days DST-STUTI-ICT Workshop

SUMMARY

The prestigious one week DST-STUTI workshop entitled "A hands-on Training Program on Approaches for Screening and Characterization of Preclinical Drug Candidates" from 8th to 14th Dec 2022 was held at the Jaypee University of Information and Technology (JUIT), Solan, Himachal Pradesh. This training program was initiated and sponsored by Department of Science and Technology (DST), under the scheme Synergistic Training program Utilizing the Scientific and Technological Infrastructure (STUTI) and organized by the Institute of Chemical Technology (ICT), Mumbai. The event was coordinated by Dr. Raj Kumar of the Department of Biotechnology and Bioinformatics and practically implemented by the faculties and staff of the Department of Biotechnology and Bioinformatics, JUIT. The workshop included a total 32 participants from different regions of India including post-graduate students, Ph.D. scholars, and faculties from well-known Universities.

The theme of the workshop was 'Preclinical Drug Discovery'. Drug discovery is the process through which potential new medicines are identified. The process of modern drug discovery starts with target identification followed by *in silico* and/or *in vitro* drug candidate screening. Pre-clinical study is carried out before testing potential drugs in human clinical trials which involves extensive *in vitro* (test tube or cell culture) and *in vivo* (animal) experiments that yield preliminary efficacy, toxicity, pharmacokinetic and safety information. The potential drug candidates from pre-clinical study are pushed into well-organized clinical trials in healthy individuals and patients for further drug development. This training program largely emphasized on both *in silico* and *in vitro* experiments for

the identification of potential drug molecules at the pre-clinical stage. Seven training modules were formulated which gave hands-on experience to candidates on drug target identification, phytochemical crude extraction and analysis of metabolites from medicinal plants, characterization of phytochemicals, high throughput virtual screening, and *in vitro* cytotoxicity assay.

A seven days program included intensive training modules having a daily expert lecture session from distinguished speakers of the relevant disciplines and a session of hands-on experiments using high-end instruments. Prominent external speakers in the workshop included Dr. Omesh Kumar Bharti from State Institute of Health & Family Welfare Himachal Pradesh, Dr. Prosenjit Mondal from IIT-Mandi, Dr. Hemraj Nandanwar from CSIR-Institute of Microbial Technology, Dr. Mahesh Kulharia from Central University of Himachal Pradesh, Dr. Shamsher Singh Kanwar and Dr. Wamik Azmi from Himachal Pradesh University, Dr. Rajnish Sharma from YSP UHF Nauni, Dr. Inderjeet Kaur from Central University of Haryana, and an industry expert Dr. Umender Sharma from CorMic Biotechnologies Pvt Ltd. Internal speakers included Dr. Raj Kumar, Dr. Hemant Sood, Dr. Udayabanu M., and Dr. Gopal Singh Bisht from the Department of Biotechnology and Bioinformatics, JUIT.

Overall, the participants enhanced their skills on key instruments including RT-PCR, HPLC, Fluorescent microscope, Atomic Absorption Spectroscopy, ELISA reader, UV spectroscopy, and viscometer etc. The workshop was accomplished with its goal of imparting sufficient hands-on experience to the candidates for understanding and executing the process of preclinical drug candidate screening for the discovery of new drugs.

Inauguration & Day-1 (08.12.2022)

The program started with the inauguration ceremony on 8th Dec 2022, in the divine presence of chief guest Padma Shree awardee Dr. Omesh Kumar Bharti, State Epidemiologist, State Institute of Health & Family Welfare, Parimahal, Shimla, Himachal Pradesh. The dignitaries on the dais included honorable Vice chancellor of JUIT Prof. Rajendra Kumar Sharma, Dean of Academics Prof. Ashok Kumar Gupta, and Registrar of JUIT Maj. Gen Rakesh Bassi. The inaugural function observed the presence of more than 60 persons including the Head of the Department of Biotechnology and Bioinformatics Prof. Sudhir Kumar, Head of the Department of Physics and Materials Science Prof. Dr. P.B. Barman, Head of the Department of Humanities and Social Sciences Dr. Amit Srivastava, faculty, staff, and students. The inauguration session was started by lamp lighting and paying a tribute to the Goddess of knowledge, with a beautifully performed Saraswati Vandana. Prof. Rajendra Kumar Sharma declared the event open and embraced the presence of chief guest Dr. Omesh Kumar Bharti with a bouquet. Prof. Rajendra Kumar Sharma addressed the audience with his inspiring words of brilliance. Prof. Sudhir Kumar introduced the Department of Biotechnology and Bioinformatics to the participants. Dr Raj Kumar formally introduced the event details to the audience. The inauguration was followed by a High Tea at the Mughal Gardens, where participants had a chance to befriend and interact to the Keynote Speakers and JUIT faculty.

The theme of first day was "Target identification and validation". First technical session was proceeded by a talk of Dr. Omesh Kumar Bharti on "Breaking the barriers to introduce Intra-dermal ARV". He discussed his research on alternate and affordable treatment for rabid dog bite and. He also discussed the long self-funded research efforts and his journey when World Health Organization

reviewed their technique and approved it as a low cost anti-rabies treatment protocol. He emphasized on other possibilities of low cost Anti-rabies vaccination in India. First session was followed by the talk of Dr. Raj Kumar the topic of "Strategies for drug designing". He discussed various stages and processes involved in a drug discovery project. He emphasized the importance of computational methods in cost effective and time saving drug discovery strategies. He also discussed the drug repurposing efforts and presented his research work on a very popular topic of COVID-19 treatment. Participants showed great interest in these lectures and put up several queries to the keynote speakers.

The lecture sessions were followed hands-on training session coordinated by Dr. Jata Shankar of the Department of Biotechnology and Bioinformatics, JUIT. The participants learned important practical steps in operating RT-PCR. The participants ran their samples and understood the importance and its implementations in the COVID-19 diagnostics.













Day-2

2nd day of DST-STUTI-ICT workshop started with the theme "Plant tissue culture for secondary metabolites production from medicinal plants". The first technical session of the day was proceeded by a talk of Dr. Prosenjit Mondal, Associate Professor, School of Basic Sciences, IIT Mandi on the topic of "A new strategic plan to combat diabetes". He explained the pathophysiology of type 2 diabetes mellitus. He presented his important research on non-peptidic Glucagon-Like Peptide-1 Receptor agonists for anti-obesity and anti-diabetes therapeutics. First session was followed by the talk of Dr. Hemant Sood, Associate Professor, Department of Biotechnology and Bioinformatics, JUIT. Dr. Sood her research on "Production of Medicinal Compounds from Endangered and Commercially Important Medicinal Plants of Himalayas through Cell and Tissue Culture Technologies". She emphasized on the strategies for the production of medicinally important metabolites from Himalayan herbs using plant tissue culture techniques. The lecture sessions were followed hands-on training session coordinated again by Dr. Hemant Sood. The session gave hands-on training on plant tissue culture techniques to the participants. Participants learned and practiced plant tissue culture maintenance and callus culturing technique. They also visited the green house facility where plants are subjected to hardening before transfer to actual fields.

<u>Day-3</u>

The theme of first day was "Crude extraction and analysis of metabolites from medicinal plants". The first technical session of 2nd day was proceeded by a talk of Dr. Hemraj Nandanwar, Chief Scientist, CSIR-Institute of Microbial Technology,

Chandigarh. His talk was on the topic "Triedecaptin M: A preclinical candidate against colistin resistant Gram negative bacteria". He emphasized on various important strategies for developing drugs against multidrug resistant microbes. Dr. Nandanwar's talk was followed by the speech of Dr. Deepak Kumar, Professor, School of Pharmaceutical Science, Shoolini University, Himachal Pradesh. His topic of speech was "Design, synthesis, characterization of heterocyclic compounds and their biological activity". Dr. Kumar presented his vast research in the domain of pharmaceutical chemistry, screening, synthesis, and biological testing of small molecules again various pathologies. The lecture sessions were followed hands-on training session coordinated by Dr. Gopal Singh Bisht of the Department of Biotechnology and Bioinformatics, JUIT. This session provided hands-on training to the participants on High-performance liquid chromatography (HPLC).

Day-4

The theme of Day-4 was "High throughput virtual screening" for identification of potential lead compounds against important drug targets. The first technical session proceeded by a talk of Dr. Mahesh Kulharia, Associate Professor & Director, Centre for Computational Biology & Bioinformatics, CUHP, Himachal Pradesh. He gave an expert talk on the topic "Computer Aided Drug Discovery". Dr. Kulharia discussed various computational techniques used for virtual screening and prioritization of potential molecules from synthetic chemical databases. First session was followed by the talk of Dr. Rajnish Sharma, Associate Professor & Head, Department of Biotechnology, YSP UHF Nauni, Himachal Pradesh. He presented his important work on the topic "Biotechnological interventions in

medicinal plants: Conservation and bioactive compound extraction". This lecture was helpful to understand the origin of natural compounds and their extraction from various medicinal plants. The lecture sessions were followed hands-on training session coordinated by Dr. Raj Kumar and Dr. Tiratha Raj Singh of the Department of Biotechnology and Bioinformatics, JUIT. The participants had hands-on experience on handling molecular modeling software such as Chimera, AutoDock, and Discovery Studio. Participants also learned to perform virtual screening of compound library using molecular docking simulation experiment.

<u>Day-5</u>

The Day-5 started with the theme "*In vitro* screening: Cytotoxicity assay" of potential drug molecules. The first technical session of was proceeded by a talk of Dr. Shamsher Singh Kanwar Professor, Department of Biotechnology, Himachal Pradesh University, Shimla. He talked about the application of MTT assay for measuring cell metabolic activity. First session was followed by the talk of Dr. Udayabanu M., Associate Professor, Department of Biotechnology and Bioinformatics, JUIT. His speech had a title "Quercetin Attenuates Neurological Complications Associated with Chronic Diabetes". He emphasized on utilization of various plant metabolites in treatment of several diseases including diabetes and neurological disorders. The lecture sessions were followed hands-on training session coordinated again by Dr. Udayabanu. Participants learned basics of animal cell culture handling, and obtained hands-on training on fluorescent microscope handling.

<u>Day-6</u>

Day-6 started with the theme of "*In vitro* screening & antimicrobial assay". The first technical session of 2nd day was proceeded by a talk of industry expert Dr. Umender Sharma, Founder, CorMic Biotechnologies Pvt Ltd., Himachal Pradesh. The topic of his speech was "Genetic validation of drug targets in Mycobacterium tuberculosis". Dr. Sharma discussed various challenges and potential medications to combat tuberculosis in India. First session was followed by the talk of Dr. Gopal Singh Bisht of the Department of Biotechnology and Bioinformatics, JUIT. Dr. Bisht gave a very interesting talk on the topic "Road map for patent creation in drug discovery". He discussed several criteria and requirements for securing the intellectual property right in drug discovery field. The lecture sessions were followed hands-on training session coordinated by Dr. Saurabh Bansal, Dr. Jitendraa Vashistt, and Dr. Rahul Shrivastava of the Department of Biotechnology and Bioinformatics, JUIT. The participants received hands-on training on instruments such as Plate reader and UV visible spectrometer.

<u>Day-7</u>

The theme of Day-7 was "Nano-formulations and nanomedicines". The first technical session of final day was proceeded by a talk of Dr. Wamik Azmi, Professor & Chairperson, Department of Biotechnology, Himachal Pradesh University, Shimla. He delivered an excellent talk on the topic of "Nanopharmaceuticals and nanomedicines". He discussed the importance and application of nanomaterials in drug delivery strategies. The final lecture of the workshop entitled "Deciphering the fundamental pathways associated with calcium dependent protein kinases (CDPKs) in Plasmodium falciparum at blood stages",

was given by Dr. Inderjeet Kaur, Assistant Professor, Department of Biotechnology, Central University of Haryana, Jant-Pali, Mahendergarh, Haryana. Dr. Kaur presented her research in malaria, post translational modifications, mass spectrometry based proteomics to study PTMs, studying phosphorylation for possible malaria treatments. The lecture sessions were followed hands-on training session coordinated by Prof. Sudhir Kumar, Dr. Abhishek Chaudhary, and Dr. Poonam Sharma of the Department of Biotechnology and Bioinformatics, JUIT. The participants received hands-on training on instruments such as Atomic Absorption Spectroscopy and Viscometer.

Valedictory ceremony

On Wednesday, December 14, 2022, the enriching journey through the "Hands-on Training Program on Approaches for Screening and Characterization of Preclinical Drug Candidates" reached its conclusion as the curtains were drawn on this transformative experience. The valedictory function, coordinated by the event's cocoordinators Dr. Udayabanu M., Dr. Shikha Mittal, Dr. Ashok Kumar Nadda, and Dr. Rahul Shrivastava, marked the ceremonial close of this impactful program. During this training program, distinguished keynote speakers were honored for their contributions with certificates, traditional Himachali caps, mufflers, and mementos, symbols of gratitude for sharing their invaluable knowledge throughout the program. The event enjoyed the esteemed presence of Prof. Rajendra Kumar Sharma, the Honorable Vice Chancellor of JUIT, who bestowed his blessings upon all workshop participants. His words resonated with the participants, urging them to preserve the memories and carry forward the profound learnings acquired during the training to propel progress in their research endeavors. Acknowledging the significance of the program, Prof. Sudhir Kumar extended his appreciation to the organizing committee for creating a platform where experts from diverse fields

could unite to impart their ideas and research to the eager students. His encouraging words prompted participants to integrate the newfound knowledge into their lives, fostering a meaningful impact. Dr. Raj Kumar extended the Vote of Thanks, acknowledging the guests of the valedictory session, the faculty of the University, the dedicated staff involved in the workshop's execution, the enthusiastic participants, and the student volunteers, whose combined efforts culminated in the success of this program.

This immersive training provided participants with a unique opportunity to delve into the intricate realm of drug discovery and development, with a primary focus on the crucial phases of screening and characterization of pre-clinical drug candidates. Unlike a mere theoretical discourse, this training was a dynamic platform for hands-on exploration and experiential learning. Guided by our esteemed faculty of experts, participants navigated the intricate process of identifying potential drug candidates and meticulously scrutinizing their pharmacological attributes. From initial compound selection to the application of cutting-edge methodologies for characterization, attendees were exposed to the latest advancements and best practices in this evolving field. The lessons learned in this workshop will undoubtedly serve as guiding lights in the future endeavors of the participants, as they strive to bring forth safer and more effective medications for the betterment of global health.