



DEPARTMENT OF CHEMISTRY

Brief Report

A Two-Week Faculty Development Program

on

Computational Tools for Drug Discovery: An Approach towards Attainment of Sustainable Development Goals

From June 06-18, 2022

The Department of Chemistry under the guidance of **Prof. Abdul Rahman Khan**, Dean Faculty of Science and Head, Department of Chemistry has organized a Two-Week Online (Face to Face) Faculty Development Program (FDP) on “**Computational Tools for Drug Discovery: An Approach Towards Attainment of Sustainable Development Goals**” from **June 6-18, 2022**. The FDP was aimed at deciphering various computational tools and methodologies for their effective applications in drug design such as de novo design, molecular docking, molecular similarity calculation, and sequence-based virtual screening.

The FDP was attended by **229 participants** not only from various states of India but also from other countries.

The Inaugural session was graced by the presence of **Prof. G.P.S. Raghava**, Head, Department of Computational Biology, Indraprastha Institute of Information Technology (IIIT), New Delhi. Prof. Raghava is a recipient of **Shanti Swarup Bhatnagar Award in Biological Science**, 2008 and Fellow of National Academy of Sciences (F.N.A.Sc). Prof Raghava captivated the participants during his session on **Open source software and repositories for drug discovery**. During the two-week program, reputed scientists and academicians from **CSIR-CDRI, CSIR-CIMAP, Central Universities, IIIT, Allahabad and Monash University, Australia** disseminated current knowledge on different computational aids and strategies useful for drug designing and discovery. For the valedictory session, **Prof. Shandar Ahmad**, School of Computational and Integrative Sciences, JNU, New Delhi was the keynote speaker. Prof. Shandar Ahmad has received grants from various reputed national and international funding agencies. Prof. Shandar Ahmad has shared his expertise on the topic **AI and machine learning in biomolecular systems**.

For making the FDP successful, the conveners; **Dr. Minaxi B. Lohani & Dr. Malik Nasibullah**, co-conveners; **Dr. Naseem Ahmad & Dr. Firoz Hassan** and all the organizing committee members have given significant contributions.

All the sessions of the FDP were interactive and appreciated by the participants who were academicians, and research scholars of different scientific backgrounds like Chemistry, Biosciences and Pharmaceutical Sciences.

Highlights of the FDP

Total Registered Participants = **229**

Participants successfully completed the program = **218**

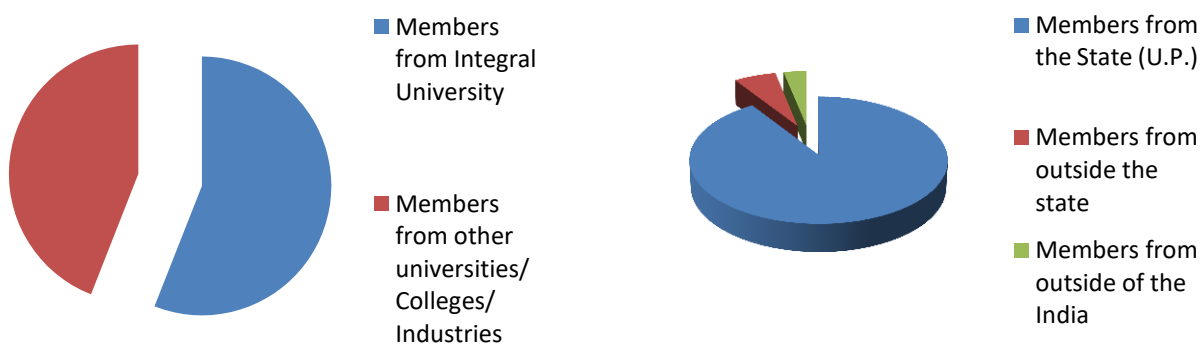
Participants from Integral University, Lucknow = **122**

Participants from other universities/ colleges = **96**

Participants from outside of the India = **07**

More than 60 hours online active engagement through content based learning on Google meet and ili (LMS)

Statistical Analysis of the Participants who have successfully completed the program



Sessions of the Program

Week-1

Inaugural Session (6th June, 2022): The welcome address was delivered by **Prof. Abdul Rahman Khan**, Dean, Faculty of Science and Head, Department of Chemistry followed by the address of the Honorable Vice-Chancellor, **Prof. Javed. Musarrat**, who congratulated the department for organizing the FDP on a very relevant topic in today's time.

Session I (6th June, 2022): The resource person for the first session was **Prof. G. P. S. Raghava**, Head, Department of Computational Biology, Indraprastha Institute of Information Technology Delhi. **Prof. Raghava** in lecture deliberated on the importance of open source software and repositories for drug discovery. The session was ably managed by **Dr. Minaxi B. Lohani, Convener** of the FDP.

Session II (7th June, 2022): **Dr. Saleem Javed**, Associate Professor, Department of Chemistry Institute of H. Science, Khandari, Dr. B. R. Ambedkar University, Agra was the resource person on the second day of the programme. In his talk, he dwelled upon the Synthesis, Spectroscopic and Quantum Chemical Investigation of Medicinally important heterocyclic compounds. The session was well managed by **Dr. Qazi Inamur Rahman**.

Session III (8th June, 2022): The third session was graced by **Dr. Md. Ataul Islam**, Senior Computational Chemist, 3BIGS Omicscore, Bangalore, India. Dr. Islam enlightened the participants on Pharmacoinformatics as an important computational approach in drug discovery. **Dr. Iqbal Azad** ably managed the session.

Session IV (9th June, 2022): On the fourth day of the FDP, **Dr. Imran A. Khan** from the Department of Chemistry, School of Chemical and Life Science, Jamia Hamdard University, New Delhi. The session was ably managed by **Dr. Nafees Ahamd.**

Session V (10th June, 2022): The resource person for the fifth session of the FDP was **Dr. Yusuf Akhter**, Assistant Professor, Department of Biotechnology, School of Life Science, BBAU, Lucknow. Dr. Akhter discussed his work on drug resistance mechanisms in Mycobacterium tuberculosis, molecular diversity to evolution through computational approach. The session was well managed by **Dr. Firoj Hassan.**

Quiz I (11th June, 2022): The first quiz was made available for the participants on 11th June at 12:00 pm. The quiz consisted of 20 questions.

Week-2

Session VI (13th June, 2022): The resource person for the sixth session was **Dr. Feroz Khan**, Senior Principal Scientist, Metabolic & Structural Biology, CSIR-CIMAP, Lucknow. Dr. Khan introduced the concept of QSAR Modeling, Machine Learning methods and application for Lead identification and optimization. The session was ably managed by **Dr. Qazi Inamur Rahman.**

Session VII (14th June, 2022): **Dr. Mohd. Imran Siddiqi**, Senior Principal Scientist, Biochemistry and Structural Biology, CSIR-CDRI, Lucknow was the expert speaker for the seventh session of the FDP. **Dr. Imran** discussed the recent trends in Computer-Aided Drug Design and Virtual Screening for Real Molecules of therapeutic relevance. The session was well managed by **Dr. Naseem Ahamd.**

Session VIII (15th June, 2022): the resource person for the day was **Dr. Nidhi Mishra**, Associate Professor, Department of Applied Chemistry, IIT, Allahabad. Dr. Nidhi very aptly explained the applications of QSAR, molecular docking and simulation in drug discovery and their exploration in Natural products for the development of novel drug compounds. The session was managed by **Dr. Tahmeena Khan**, on behalf of the organizing committee.

Session XI (16th June, 2022): **Dr. Santosh Panjekar**, Adjunct Faculty member, Dept. of Biochemistry and Molecular Biology, Monash University, Australia. Dr. Panjekar delivered his talk on Structural Biology and Drug Discovery. The session was well-managed by **Dr. Daraksha Bano.**

Session X (17th June, 2022): The guest speaker for the valedictory session was **Prof. Shandar Ahmad**, School of Computational and Integrative Sciences, JNU, New Delhi. Prof. Ahmad shared his expertise on AI and machine learning in biomolecular systems. The session was managed by **Dr. Malik Nasibullah**, convener of the FDP.

Quiz II (18th June, 2022): The second quiz was made available for the participants on 18th June at 12:00 pm. The quiz consisted of 20 questions.

Overall the Faculty Development Program was a great success. All the sessions were very informative and well-attended by participants from different streams.

Boucher of the Program

RESOURCE PERSONS

 Prof. Ravindra Kumar Associate Professor Department of Chemistry Integral University Lucknow-226002 18 th June 2022	 Dr. Sandhya Prasad Department of Chemistry Integral University Lucknow-226002 18 th June 2022	 Dr. Sandhya Prasad Department of Chemistry Integral University Lucknow-226002 18 th June 2022
 Dr. Anshu A. Kumar Associate Professor Department of Chemistry Integral University Lucknow-226002 18 th June 2022	 Dr. Pooja Agrawal Department of Chemistry Integral University Lucknow-226002 18 th June 2022	 Dr. Pooja Agrawal Department of Chemistry Integral University Lucknow-226002 18 th June 2022
 Dr. Anshu A. Kumar Associate Professor Department of Chemistry Integral University Lucknow-226002 18 th June 2022	 Dr. Anshu A. Kumar Associate Professor Department of Chemistry Integral University Lucknow-226002 18 th June 2022	 Dr. Anshu A. Kumar Associate Professor Department of Chemistry Integral University Lucknow-226002 18 th June 2022
 Prof. Dr. Nasir Ahmad Head Department of Chemistry, Integral University Lucknow-226002 18 th June 2022		

FOR ANY QUERIES PLEASE CONTACT:
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DEPARTMENT OF CHEMISTRY
IS ORGANIZING

TWO WEEK
FACULTY DEVELOPMENT PROGRAM (FDP)
ONLINE FACE TO FACE

ON
COMPUTATIONAL TOOLS FOR
DRUG DISCOVERY:
AN APPROACH TOWARDS ATTAINMENT
OF SUSTAINABLE DEVELOPMENT GOALS

JUNE 6 - 18, 2022





Integral University
Lucknow-226002

100 Years
11th Group
25th Anniversary
178th Anniversary
12,000+ Students
2200+ Faculty
1000+ Staff
10,000+ Alumni

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25th Anniversary
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178th Anniversary
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2200+ Faculty
1000+ Staff
10,000+ Alumni

CHIEF PATRONS	PATRONS	
 Prof. Dr. Nasir Ahmad Head, Department of Chemistry	 Dr. Sandhya Prasad Head, Department of Chemistry	 Prof. Dr. Nasir Ahmad Head, Department of Chemistry
CO-PATRONS		
 Dr. Anshu A. Kumar	 Dr. Pooja Agrawal	 Dr. Anshu A. Kumar
 Dr. Anshu A. Kumar	 Dr. Pooja Agrawal	 Dr. Anshu A. Kumar
CONVENERS		
 Dr. Anshu A. Kumar	 Dr. Pooja Agrawal	 Dr. Anshu A. Kumar
 Dr. Anshu A. Kumar	 Dr. Pooja Agrawal	 Dr. Anshu A. Kumar
ORGANIZING COMMITTEE		
 Dr. Anshu A. Kumar	 Dr. Pooja Agrawal	 Dr. Anshu A. Kumar
 Dr. Anshu A. Kumar	 Dr. Pooja Agrawal	 Dr. Anshu A. Kumar

IMPORTANT INSTRUCTIONS

1. Registration Fee: Rs. 1000/-
2. Fee to be paid by the candidate at the time of registration.
3. Registration form will be sent to the candidate after successful registration.

Registration Form Link: <https://forms.gle/CoCvBL4x3OwRCK79>

Sample Certificate



INTEGRAL UNIVERSITY
LUCKNOW - INDIA

75th Anniversary
आमरी अमृत महोत्सव



INSPIRING EXCELLENCE
Celebrating
24 years of
EXCELLENCE

Certificate of Participation

Certificate Number: 62becb57-3368-4b3f-af73-b76f40e3bed3

This is to certify that

Dr. Naseem Ahmad, Integral University, Lucknow
has successfully completed two-week Faculty Development Program
On
Computational Tools for Drug Discovery:
An Approach towards Attainment of Sustainable Development Goals
Organized by

Department of Chemistry

From June 06 - 18, 2022


(Dr. Malik Nasibullah)
Convener
Faculty Development Program


(Dr. Minaxi B. Lohani)
Convener
Faculty Development Program


(Prof. Abdul Rahman Khan)
Dean, Faculty of Science &
Head, Department of Chemistry

