

ONE-WEEK ONLINE  
**FACULTY DEVELOPMENT PROGRAMME**

Computational Approach to  
**Drug Discovery**

**2 Aug - 7 Aug, 2021**

Live sessions : 2:00 - 5:15 pm



Ministry of Education  
Government of India



Hansraj College



Deshbandhu College



Pathfinder Research  
and Training Foundation

**DESHBANDHU COLLEGE**

(Under the aegis of DBT Star College Scheme & DBC i4 Centre)

and

**CENTER FOR BIOINFORMATICS,  
COMPUTATIONAL AND SYSTEMS BIOLOGY**

**Pathfinder Research and Training Foundation**

*in collaboration with*

**MAHATMA HANSRAJ FACULTY DEVELOPMENT CENTRE**

**HANSRAJ COLLEGE**

(A Centre of MoE, Govt. of India under PMMMNMTT Scheme)



### About Deshbandhu College

Established in 1952, Deshbandhu College, is the oldest amongst all colleges under University of Delhi, South Delhi having more than 5000 students taking admission each year. Ranked 44<sup>th</sup> in Science in the *India Today 2021* survey, it boasts of having nearly 200 research publications in SCI/SCOPUS/UGC-CARE indexed international and national referred journals and has received more than Rs. 75,00,000/- in research grants in the year 2019-20. Recently, the college has been awarded with “DBT-Star College” Scheme by Department of Biotechnology, under which *i4 Centre* (Student Research Centre) was established in the college for interdisciplinary research. The college has 4 university approved Research laboratories with more than 20 PhD scholars and 2 Post-Doctoral Research fellows engaged in full-time research activities. It has the largest collection of books and journals, print and digital, in its library, ranked 1<sup>st</sup> by DRDO. The college has recently developed about 4 acres of green landscape offering a variety of more than 35 species. The college campus is fully environment friendly having installed solar panels to maximize alternate power resource management.



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### About PMMMNMTT

The Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching emphasizes the need to change the role and working of a teacher from being a mere disseminator of information and knowledge to the one who advances the frontiers of existing knowledge by actively developing and creating new insights into diverse social and physical phenomena.



### About Center for Bioinformatics, Computational and Systems Biology, PRTF

The Center for Bioinformatics, Computational and Systems Biology functioning under the aegis of Pathfinder Research and Training Foundation is a

state-of-the-art platform for researchers to perform wide range of research activities related to drug discovery, NGS analysis, metagenomics, structural biology, large scale cell imaging, machine learning and engineering software development. The mission of the center is to excel and lead in scientific research, training and in creating a new, broad and interdisciplinary view of computational and systems biology.



### About Hansraj College

Hansraj College is one of the largest constituent colleges of the University of Delhi and has been ranked as one of the top five colleges for science, arts and commerce several times in the last decade. The faculty and students of the college have contributed immensely to the fields of academics, sports and culture. The college faculty is dedicated towards the growth and development of the institution academically and administratively and constantly thrive for excellence. Hansarians have been placed in diverse professions and services worldwide and are bringing fame and laurels to the institution.

## About The Programme

In drug discovery, bioinformatics tools enable the identification of potential compounds of therapeutic interest by predicting the ligand-target interactions at a molecular level. This faculty development programme is designed to provide inclusive training on the application of computational drug discovery approaches against various diseases through hands-on training and developing research oriented skills. The course includes step-by-step lectures/hands-on/tutorials to the methodologies associated with the included topics.

### Programme highlights:

- Protein structure, databases and visualization
- Protein 3D structure prediction and validation
- Basic concepts of drug discovery
- Structure based virtual screening
- Molecular docking
- Protein-ligand Complex minimization
- Molecular interaction analysis
- QSAR Modeling
- Pharmacophore modeling
- Ligand based screening

## Organizing Team

### MAHATMA HANSRAJ FACULTY DEVELOPMENT CENTRE

**Prof. (Dr) Rama**

Principal, Hansraj College  
Chairperson, MHRFDC

**Dr. Jyoti Bhola**

Coordinator, MHRFDC

**Mr. Ashutosh Yadav**

Dy. Coordinator, MHRFDC

**Dr. Archana Singh**

FDP Coordinator, Hansraj College

### DESHBANDHU COLLEGE

**Prof. (Dr) Rajiv Aggarwal**

Principal, Deshbandhu College &  
Chairperson, DBC i4 Centre

**Dr. Indrakant K. Singh**

FDP Convenor &  
Head, DBC i4 Centre

**Dr. Aditya Saxena**

(IQAC, Coordinator)

**Members, Organising Committee**

Dr. Moses Rinchui N.

Dr. Preeti Karwal

### CENTER FOR BIOINFORMATICS COMPUTATIONAL AND SYSTEMS BIOLOGY



Prof. G P S Raghava  
IIIT-Delhi

Honorable  
keynote  
speaker

**Dr. Vivek Dhar Dwivedi**

Scientist

**Dr. Shiv Bharadwaj**

Visiting Scientist

**Dr. Avinash Mishra**

Visiting Scientist



Date	Topics	Time	Scientist's Name
<b>02-08-2021</b> <b>(Monday)</b>	Inauguration, Welcome address and instructions session	03:00 PM – 4:00 PM	(Login will start at 02:00 PM)
	Bioinformatics and its applications <b>(Keynote Inaugural Lecture)</b>	04:00 PM – 5:30 PM	<b>Prof. GPS Raghava</b>
<b>03-08-2021</b> <b>(Tuesday)</b>	Live session –I Drug Discovery Pipeline: An Introduction	03:00 PM – 4:00 PM	<b>Dr. Shiv Bharadwaj</b>
	Live session –II Overview on Protein structure, databases and visualization & Hands on Practice session: sequence and protein structure database (Live session –I)	04:00 PM – 6:00 PM	<b>Dr. Vivek Dhar Dwivedi</b>
<b>04-08-2021</b> <b>(Wednesday)</b>	Live session –I Protein 3D structure prediction and validation (session –I)	03:00 PM – 4:00 PM	<b>Dr. Shiv Bharadwaj</b>
	Live session –II Hands on Practice session: 3 D protein structure prediction and Validation	04:00 PM – 6:00 PM	<b>Dr. Vivek Dhar Dwivedi</b> <b>Dr. Shiv Bharadwaj</b>
<b>05-08-2021</b> <b>(Thursday)</b>	Live session –I Molecular Docking	03:00 PM – 4:00 PM	<b>Dr. Vivek Dhar Dwivedi</b>
	Live session –II Hands on Practice session: molecular docking & Molecular interactions analysis (session –II)	04:00 PM – 6:00 PM	<b>Dr. Vivek Dhar Dwivedi</b> <b>Dr. Shiv Bharadwaj</b>
<b>06-08-2021</b> <b>(Friday)</b>	Live session –I & II Lecture and Hands on Practice session: QSAR Modeling	03:00 PM – 6:00 PM	<b>Dr. Avinas Mishra</b>
<b>07-08-2021</b> <b>(Saturday)</b>	Live session –I Hands on Practice session: Structure Based Virtual Screening	03:00 PM – 4:00 PM	<b>Dr. Vivek Dhar Dwivedi</b>
	Live session –II Hands on Practice session: Pharmacophore Modeling and Ligand Based Virtual Screening	04:00 PM – 5:00 PM	<b>Dr. Vivek Dhar Dwivedi</b> <b>Dr. Shiv Bharadwaj</b>
	Concluding Remarks, Valedictory Session & Feedback	05:00 PM – 6:00 PM	

**Note:**

1. Library hours: 1:00 PM to 2:00 PM (Everyday)
2. Practice and revision (Online): 2:00PM to 3:00PM (Everyday)
3. Live sessions: 3:00PM to 6:00PM (Everyday)
4. Software Installations/Assessment and Evaluation: 6:30 PM to 7:30PM (Everyday).

## REGISTRATION DETAILS

Interested participants are requested to follow the steps mentioned below in order to register for the FDP:

Participants are required to pay the registration fee of **Rs. 500** via **NEFT/IMPS/UPI** to the following account:

<b>Account:</b>	<b>Principal, Hansraj College, FDC</b>
<b>Bank:</b>	<b>Canara Bank, Hansraj College, Delhi</b>
<b>Type of Account:</b>	<b>Savings</b>
<b>Account number:</b>	<b>2848101019873</b>
<b>IFSC:</b>	<b>CNRB0002848</b>

- **NOTE: Fee is Non-Refundable**
- Pre-registration to the programme is through **online** mode only.
- Participants are required to fill the registration form using the following link. (Please ensure that you have payment proof before filling up registration form)
- Registration link: <https://bit.ly/3kuLC3R>
- The **last date** for registration is **30<sup>th</sup> July 2021**.
- **Participants** will be informed by **31<sup>st</sup> July 2021**.
- Attendance norms are strict. Participants are required to clear the assessment component for getting the **e-certificates**.
- Further details will be communicated to the registered participants.
- **ELIGIBILITY:** The programme is **interdisciplinary\*** and is open to all interested participants. All faculty members (**Permanent/ Temporary/ Adhoc/ Guest**) and **Research Scholars** from any university/college are eligible to participate.

(\*From the department of *Biological Science/ Physical Science/ Chemical Science/ Environmental Science/ Mathematical and Computer Sciences*)