



RBVRR Women's College of Pharmacy

Barkatpura, Hyderabad, 500027, (T.S)

Accredited by NAAC, Approved by the PCI & Affiliated to Osmania University, Recognised under section 2(f) of the UGC Act 1956



In Collaboration With NIZAM College (Autonomous)

Basheerbagh, Hyderabad, 500001, (TS)



Organizing Certificate Course

On

Computational Tools in Drug Design and Development

TARGET AUDIENCE

Students & Researchers
Academicians & Educators
Industry Professionals

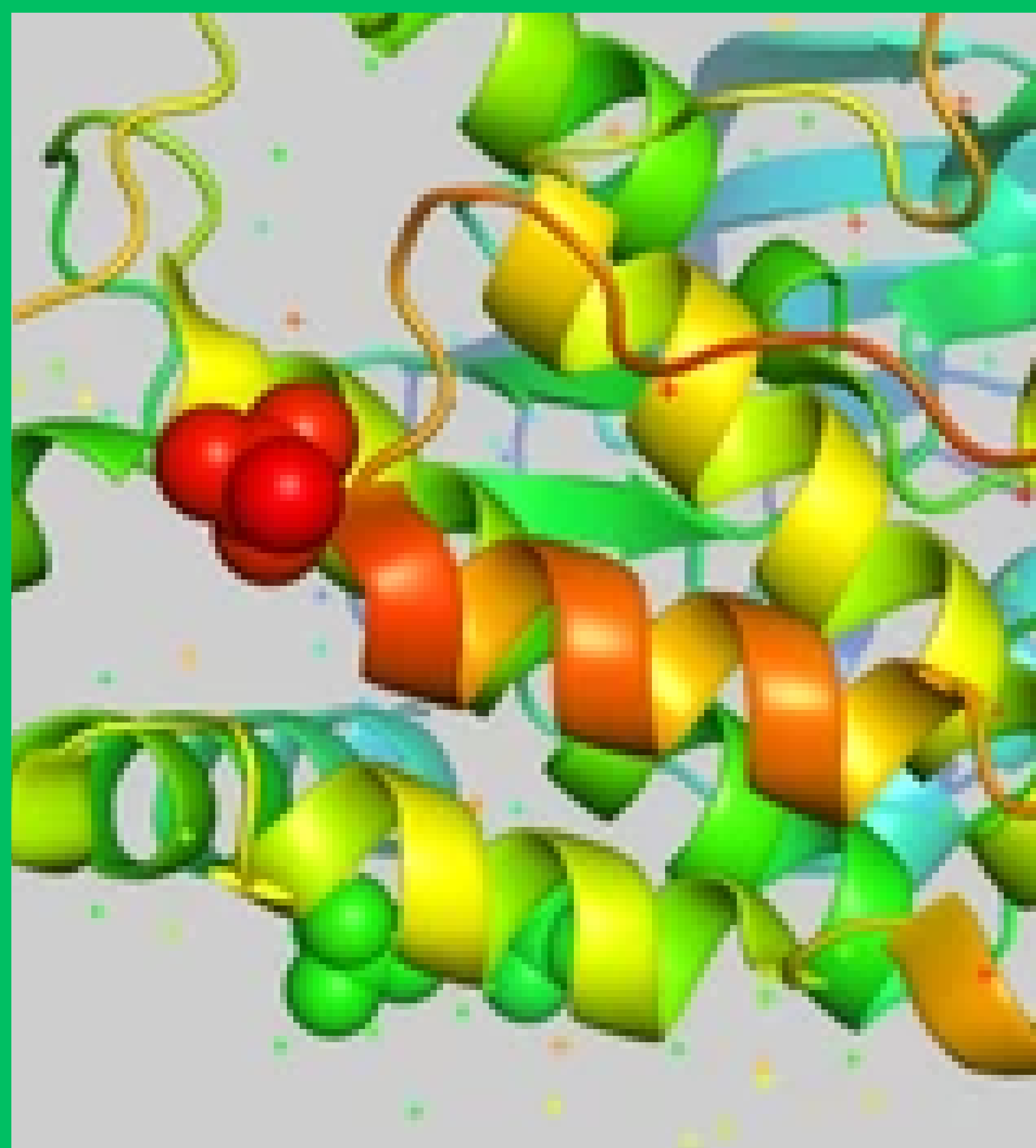
REGISTRATION LINK

<https://forms.gle/cfgaMNiuJocZbq3J9>

REGISTRATION FEE

Students : 1000

Faculty & others: 1500



24th - 29th March 2025

Last Date for Registration

22nd March 2025

MAXIMUM No. of Participants: 40

About RBVRR Women's College of Pharmacy

RBVRR Women's College of Pharmacy, established in 2006 under the Hyderabad Mahila Vidhya Sangam, is driven by the visionary leadership of its Founder Principal, Prof. M. Sumakanth. The college is dedicated to empowering girl students through education and offers spacious classrooms, state-of-the-art laboratories, a well-equipped seminar hall, a conference room, and a library stocked with a wide range of the latest textbooks, reference materials and digital library

The college is offering the following programmes:

B. Pharmacy (100)

Pharm. D (32)

M.Pharmacy (Pharmaceutics, Pharm. Analysis and Pharmacology).

VISION: To be a National Women Pharmacy Professional leader in transforming lives through innovative, vigorous and compassionate approach to Pharma education.

MISSION: RBVRRWCP preparing and empowering girl students by providing continuous awareness programmes to succeed in changing world apart from regular curriculum.

The aim of certificate course is to make aware of the availability of computational tools and softwares to enhance the drug discovery process by leveraging in silico techniques to identify, optimize and validate potential drug candidates efficiently. These tools integrate bioinformatics, cheminformatics and molecular modeling.

OBJECTIVES

- Understand the Role of Computational Methods
- Master Molecular Docking and Virtual Screening
- Interpretation of Protein-Ligand Interactions
- Bridge Computational and Experimental Drug Discovery
- Train with tools like AutoDock, Gemdock and PyMOL
- Databases and computational methods to analyze chemical and biological data
- Enhance decision-making in drug design with *in silico* techniques



About Nizam College (Autonomous)



Department of Chemistry is the largest Department of Nizam College. B.Sc program was started way back in 1918 and M.Sc. in 1967. It is the first department to have Chemistry PG program outside the University Campus. The Alumni include stalwarts like Prof. T. Navaneeth Rao, Prof. M. M. Taqui Khan. The Department offers UG (5 combinations), PG (Physical chemistry with Polymer Chemistry as Elective and Inorganic chemistry with Bioinorganic Chemistry as Elective), PG (Organic chemistry with medicinal chemistry), PG (Pharmacoinformatics), M.Sc Five year integrated Course in Chemistry (FYIC). In Osmania University the Polymer Chemistry elective is offered only at Nizam College and Bioinorganic Chemistry elective is offered at Nizam college and Women's College (outside the campus). The department has strong faculty working in the fields of Bioinorganic chemistry, Cheminformatics and Molecular modeling, Spectroscopy, Synthetic chemistry and Chemical kinetics. Similar to Osmania University, the Department has also many firsts to its credit : First department to have PG program in chemistry outside the O.U. Campus, First in India to introduce molecular modeling in M.Sc. (Chemistry) curriculum.

Program Co-ordinators

Dr.M. Vijaya Bhargavi

Associate Professor & Head
Department of Pharmaceutical
Chemistry, RBVRRWCP

Dr. M. Radhika

Assistant Professor & Head
Department of Chemistry
Nizam College

Account Details

Account No: 039710011906455

IFSC Code: UBIN0803979

Union Bank of India

Narayanguda Branch, Hyd.

For Queries Contact

Mrs.Mariya Sana: 8008348994

9848054391, 9849583030

Certificate Course On Computational Tools in Drug Design and Development

Value added Course

Code: APCCC002 Credits: 4 Total No. of Hours: 30

Unit 1: Introduction to Computational Drug Design and Development (6hrs)

Drug Discovery Stages: From target identification to clinical trials.
Computational Tools PyMol and databases PDB, PubChem, ChEMBL, Drug bank

Unit 2: Molecular Modeling (6 hours)

Molecular structure representation, 2D vs 3D structures, Molecular descriptors and their relevance in drug design
Energy minimization and structure optimization
Techniques used for energy minimization
Tools for structure optimization

Unit 3: Molecular Docking and Virtual Screening (6 hours)

Molecular Docking: Principles of protein-ligand docking and scoring, docking softwares.
Virtual Screening: Techniques for screening compound libraries.

Unit 4: Quantitative Structure-Activity Relationship (QSAR) Modeling (6 hrs)

Introduction to QSAR, Concept and significance in drug design,
Types of QSAR models: 2D, 3D-QSAR
Steps in QSAR modeling and Tools for QSAR modeling, Data collection and preprocessing, Descriptor selection and feature extraction, Model building and interpretation of QSAR models

Unit 5: Integration of Computational Tools in Drug Development (6 hours)

Computational approaches in lead optimization, Identifying and optimizing drug-like properties , ADMET (Absorption, Distribution, Metabolism, Excretion, Toxicity) prediction
Computational toxicology, Tools for predicting toxicity and safety

Programme Schedule

DATE	Morning Session 10:30AM-1:00PM	Afternoon Session 2:00PM-4:30PM Hands on Training
24/03/2025	Inaugural Session Prof. G. Narahari Sastry IIT-Hyderabad	Dr.M. Vijaya Bhargavi RBVRRWCP
25/03/2025	Dr. Vasundhra Bhandari NIPER, Hyderabad	Dr. V. Padmaja RBVRRWCP
26/03/2025	Dr. S. Sree Kanth VCIWU, Koti, Hyderabad	Dr. S. Sree Kanth VCIWU, Koti, Hyderabad
27/03/2025	Dr. S. Gururaj Nizam College Hyderabad	Dr. S. Gururaj Nizam College Hyderabad
28/03/2025	Prof. M. Sumakanth RBVRRWCP	Prof. M. Sumakanth RBVRRWCP
29/03/2025	Prof. M. Vijjulatha University College of Science, OU	Valedictory

Course Experts



Dr. G. Narahari Sastry
Professor
Department of Biotechnology
IIT- Hyderabad.



Dr. Vasundhra Bhandari
Assistant Professor
Department of
Pharmacoinformatics
NIPER



Dr. S. Sree Kanth
Assistant Professor (c)
Department of Chemistry
VCIWU, Koti, Hyderabad



Dr. S. Gururaj,
Assistant Professor (c)
Department of Chemistry
Nizam College.



Prof. M. Sumakanth
Principal
RBVRR Women's College
of Pharmacy



Dr. M. Vijjulatha
Professor
Department of Chemistry
University College of Science
Osmania University

