Name: Dr. Anu Manhas

Designation: Assistant Professor, Department of Chemistry, School of Technology, Pandit Deendayal Energy University, (Former PDPU), Gandhinagar, Gujarat-382426.

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Brief Bio:
The overall aim of my research work is to advance the knowledge of structure-based pharmacophore modeling approach as well as provide useful suggestion for their application in virtual screening. For this purpose, we utilize the knowledge of the pharmacophore modeling to provide an insight about the feature similarity among the selected enzyme classes and share of features among the experimentally reported inhibitors of malaria and tuberculosis. The rationale was to search for the representative pharmacophores and to provide guiding principle for the design of stringent pharmacophore that can be employed for the virtual screening to rationally design new chemical entities that could contribute in treating human diseases. In this regard, we use wide range of methods like multicomplex-based pharmacophore modeling and molecular docking, virtual screening methods like drug-likeness studies and ADMET properties, molecular dynamics simulations and free energy calculations.

TEACHING

July 2020 to present	Assistant Professor, Department of Chemistry, School of Technology, Pandit Deendayal Energy University, (Former PDPU), Gandhinagar, Gujarat-382426

PROJECTS

2 Sept 2021 to present	Student Research Program (by Pandit Deendayal Energy University)
2 Dec. 2021 to present	Teachers Associateship for Research Excellence (TARE) (by Science and Engineering Research Board)

MEMBERSHIPS

- Indian Society of Chemists and Biologists (ISCB): 1161/2022
- International Society for Computational Biology and Bioinformatics (ISCB): 37142
- Member (MRSC): 719271

EDUCATION

Jan 2016 to Feb 2020	Central University of Gujarat, Ph.D., Chemical Sciences, Gandhinagar, Gujarat, India
Aug 2014 to Jan 2016	Central University of Gujarat, M.Phil., Chemical Sciences, Gandhinagar, Gujarat, India
Aug 2011 to Jul 2013	Lovely Professional University, M.Sc., Chemistry (Hons.), Phagwara, Punjab, India
Jun 2008 to Jun 2011	Government Gandhi Memorial Science College, Bachelor of Science, Medical, Jammu, Jammu and Kashmir, India

AWARDS

Dec 2021	Awarded with Teachers Associateship for Research Excellence project by the Science and Engineering Research Board
Sept 2021	Awarded with Student Research Program project by the Office of Research and Sponsored Programs, Pandit Deendayal Energy University
July 2021	Guest of Honor and Speaker in the 2nd International Conference on Recent Trends in Computational Cancer Biology and COVID-19 (ICRTCCBC-2021)
Feb 2020	Best Oral Presentation, National Science Day, organized by School of Nano Sciences, Central University of Gujarat, India
Jul 2019	Senior Research Fellow, Department of Science and Technology- Science and Engineering Research Board (DST-SERB) (EMR/2016/003025), School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India
Apr 2018	Best Poster Presentation, National Conference on Applied Materials Science, organized by Centre for Applied Chemistry, Central University of Gujarat, India
Jul 2017	Best Oral Presentation, International Conference on Frontiers at the Chemistry-Allied Sciences Interface, organized by Centre of Advanced Study, Department of Chemistry, University of Rajasthan, Jaipur, India
Jul 2017	Junior Research Fellow, Department of Science and Technology- Science and Engineering Research Board (DST-SERB) (EMR/2016/003025), School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India
Apr 2017	Best Poster Presentation, International Conference on Drug Design, organized by Schrodinger at Jawaharlal Nehru University, India
Feb 2016	Best Poster Presentation, National Science Day, organized by School of Chemical Sciences, Central University of Gujarat, India
Mar 2015	Cleared GATE exam
Aug 2013	M.Sc. (Hons.) Chemistry Batch Topper

TEACHING

Bachelor of Technology (B.Tech)

1. Engineering Chemistry Theory (B.Tech. Sem. 1)
2. Engineering Chemistry Lab (B.Tech. Sem. 1)

Bachelor of Science (B.Sc.)

1. Organic Chemistry Lab – I (B.Sc. Hons. Sem. 5)
2. Computer Applications in Chemistry (Elective) (B.Sc. Hons. Sem. 7)
3. Quantum and Computational Chemistry (B.Sc. Hons. Sem. 8)
4. B.Sc. Project and Dissertation (B.Sc. Hons. Sem. 8)

Master of Science (M.Sc.)

1. Theoretical & Computational Chemistry Theory (M.Sc. Chemistry Sem. 2)
2. Theoretical & Computational Chemistry Practical (M.Sc. Chemistry Sem. 2)

RESEARCH INTEREST

Structure-based drug design
Ligand-based drug design
Drug-likeness studies
Molecular dynamics simulations
Free energy calculations

Structure-based/Ligand-based drug design: Identification of the important pharmacophores/ identification of the active site/ identification of the interacting molecules.

Drug-likeness filters: Lipinski's Rule of 5, Veber's Rule, ADMET properties.

Molecular dynamics simulations: Stability of newly formed complexes, Root-mean-square deviation of protein and ligand, Root-mean-square fluctuation of protein and ligand, secondary structure elements of the protein chains, To study the mechanism of action of the protein, and change that occurs during the binding of the molecule, finding out the appropriate force field, Effect of pH, etc.

Density Functional Theory: Functional group assessment, Ground state calculations, Excited state calculations, NBO calculations, Potential energy scanning curves, Ground state and Excited state energy calculations, FMO calculations, Thermal properties (Binding energy and free energy), Transition state calculations, Frequency calculations, Electrostatic potential plots, hybridization, atomic hybrid contribution,

FMO calculations: Deciphering the mechanism of sensing

Thermal properties: Anion binding affinity with the selected sensor

Energy calculations: Absorption, emission, calculate the reactivity of the molecules

RESEARCH GUIDANCE

BSc Dissertation

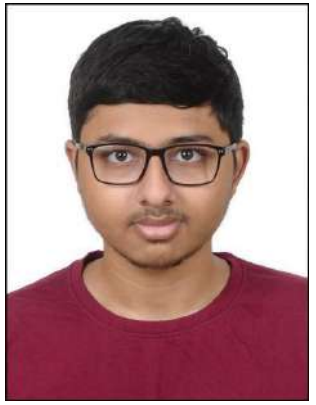
2021

Chinar Patel: Molecular Docking For The Optimization Of Hits Into Leads For Novel Drug Target Of *Plasmodium falciparum*.

Hetvi Patel: Pharmacophore Modeling In Identifying The Hits Against The Druggable Target Of *Plasmodium falciparum*.

2022

Richa Patel: Molecular Docking in drug design.



Tirth Manavadaria: Pharmacophore Modeling in drug design.

PUBLICATIONS

Journal Publications

1. **Anu Manhas***, Amar Ghosh, Yogesh Verma, Tanay Das, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2022, DOI: 10.1080/07391102.2022.2027819 **(*Corresponding Author)**
2. Amar Ghosh, **Anu Manhas***, Prakash C. Jha, *Journal of Cellular Biochemistry* 2022, DOI: 10.1002/jcb.30209 **(*Corresponding Author)**
3. Siddhi Kediya, **Anu Manhas**, Mohsin Y Lone, Prakash C. Jha, *Journal of Molecular Graphics & Modelling* 2022, 110, 108049, DOI: 10.1016/j.jmgm.2021.108049
4. Siddhi Kediya, **Anu Manhas**, Prakash C. Jha, Journal of Physical Organic Chemistry 2021, 35(1), e4283, DOI:10.1002/poc.4283
5. Ayushi Sethiya, Jay Soni, **Anu Manhas**, Prakash Chandra Jha & Shikha Agarwal, *Research on Chemical Intermediates* 2021, 47, 4477–4496, DOI:10.1007/s11164-021-04529-0
6. Soni, Jay, Nusrat Sahiba, Ayushi Sethiya, Pankaj Teli, Dinesh Kr Agarwal, **Anu Manhas**, Prakash Chandra Jha, Deepkumar Joshi, and Shikha Agarwal, *Polycyclic Aromatic Compounds* 2020, DOI: 10.1080/10406638.2020.1852277
7. Kediya, Siddhiben*, **Anu Manhas***, Mohsin Y. Lone, and Prakash C. Jha, *Journal of Molecular Structure* 2020, 129443, DOI:10.1016/j.molstruc.2020.129443 **(*Equal Contribution)**
8. **Anu Manhas***, Sujeet Kumar, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2020, 40(1), 31-43, DOI:10.1080/07391102.2020.1806110 **(*Corresponding Author)**
9. Dinesh K. Agarwal, Ayushi Sethiya, Pankaj Teli, **Anu Manhas**, Jay Soni, Nusrat Sahiba, Prakash C. Jha, Shikha Agarwal and Pradeep K. Goyal, *Journal of Heterocyclic Chemistry* 2020, 57(9), 3294-3309, DOI:10.1002/jhet.4045
10. Ayushi Sethiya, Pankaj Teli, **Anu Manhas**, Dinesh Agarwal, Jay Soni, Nusrat Sahiba, Prakash Jha & Shikha Agarwal, *Synthetic Communications* 2020, 50(16), 2440-2460, DOI:10.1080/00397911.2020.1780613
11. Nusrat Sahiba, Dinesh K. Agarwal, **Anu Manhas**, Ayushi Sethiya, Jay Soni, Prakash C. Jha & Shikha Agarwal, *Polycyclic Aromatic Compounds* 2020, DOI:10.1080/10406638.2020.1768565
12. Siddhi Kediya, **Anu Manhas**, Prakash C. Jha, *ChemistrySelect* 2020, 5(18), 5437-5450, DOI:10.1002/slct.202000550

PUBLICATIONS

Journal Publications

13. **Anu Manhas**, Saikat Dubey, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2020, 38(9), 2704-2716, DOI:10.1080/07391102.2019.1644197
14. **Anu Manhas**, Dhaval Patel, Mohsin Y. Lone, Prakash C. Jha, *Journal of Cellular Biochemistry* 2019, 120(9), 14531-14543, DOI:10.1002/jcb.28714
15. **Anu Manhas**, Mohsin Y. Lone, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2019, 37(16), 4181-4199, DOI:10.1080/07391102.2018.1540362
16. **Anu Manhas**, Mohsin Y. Lone, Prakash C. Jha, *Molecular Diversity* 2019, 23(2), 453-470, DOI:10.1007/s11030-018-9885-5
17. **Anu Manhas**, Anjali Patel, Mohsin Y. Lone, Prafulla K. Jha, Prakash C. Jha, *Journal of Cellular Biochemistry* 2018, 119(10), 8490-8500, DOI:10.1002/jcb.27075
18. Mohsin Y. Lone, Mohd Athar, **Anu Manhas**, Prakash C. Jha, Shruti Bhatt, Anamik Shah, *ChemistrySelect* 2017, 2(33), 10848-10853, DOI:10.1002/slct.201701971
19. Vijay Kumar, Mohit Chawla, Luigi Cavallo, Abdul B. Wani, **Anu Manhas**, Sukhmanpreet Kaur, Albert Poater, Hemlata Chadar, NirajUpadhyay, *Inorganica Chimica Acta* 2018, 469, 379-386, DOI:10.1016/j.ica.2017.08.064
20. Mohsin Y. Lone, **Anu Manhas**, Mohd Athar, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2018, 36(11), 2951-2965, DOI:10.1080/07391102.2017.1372313
21. **Anu Manhas**, Mohsin Y. Lone, Prakash C. Jha, *Journal of Molecular Graphics & Modelling* 2017, 75, 413-423, DOI:10.1016/j.jmgm.2017.04.025
22. **Anu Manhas**, Sivakumar P. Kumar, Prakash C. Jha, *RSC Advances* 2016, 6 (35), 29466-29485, DOI:10.1039/C6RA01071G
23. Vijay Kumar, Niraj Upadhyay, **Anu Manhas**, *Journal of Molecular Structure* 2015, 1099, 135-141, DOI:10.1016/j.molstruc.2015.06.055
24. Vijay Kumar, Simranjeet Singh, **Anu Manhas**, Joginder Singh, Sourav Singla, Parvinder Kaur, Shivika Data, Pritika Negi, Arjun Kalia, *Oriental Journal of Chemistry* 2014, 30(4), 1771-1776, DOI:10.13005/ojc/300436

PUBLICATIONS

Proceeding Publications

1. Megha Balha*, Nikunjkumar Vagadiya, **Anu Manhas*** Materials Today: Proceedings 2022, DOI: 10.1016/j.matpr.2021.12.546 **(*Corresponding Author)**
2. **Anu Manhas***, Mohsin Yousuf Lone, Prakash Chandra Jha Materials Today: Proceedings 2022, DOI: 10.1016/j.matpr.2022.02.032 **(*Corresponding Author)**

Skills / Expertise	
	Structure and ligand based drug design, Multicomplex based pharmacophore modeling, In silico virtual screening, Molecular docking, Molecular dynamics simulations, Free energy calculations (MM-PBSA), Lead identification and optimization, Homology modeling, Density Functional Theory (DFT)
Computational programs	Discovery Studio, LeadIT, Desmond, Gromacs, Gaussian, UCSF Chimera, Maestro Schrödinger, CIMminer, Chemdraw, Autodock, ArgusLab & MarvinSketch
Operating systems	Windows, Ubuntu & CentOS
Plotting tool	Grace, Excell
Document writing tools	Microsoft word, vi text editor, gedit
Reference Manager	EndNote
Graphic Tools	MS Paint & CorelDRAW
Visualization Programs	VMD, UCSF Chimera