



Assistant Professor  
Pandit Deendayal Energy University (Former PDP),  
Gandhinagar, Gujarat-382426  
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## Anu Manhas, PhD

The overall aim of my research work is to advance the knowledge of the structure-based pharmacophore modeling approach as well as provide useful suggestions for their application in virtual screening. For this purpose, we utilize the knowledge of pharmacophore modeling to provide an insight into the feature similarity among the selected enzyme classes and the share of features among the experimentally reported inhibitors of malaria and tuberculosis. The rationale was to search for representative pharmacophores and to provide a guiding principle for the design of stringent pharmacophores that can be employed for the virtual screening to rationally design new chemical entities that could contribute to treating human diseases. In this regard, we use a 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

20 Jul 2020 to present **Assistant Professor**  
Pandit Deendayal Energy University, (Formerly PDP), Gujarat-382426

## Projects

1 Jun 2022 to present **BioSolveIT Research Challenge** (by Software Development Sankt Augustin, NRW)  
2 Dec. 2021 to present **Teachers Associateship for Research Excellence (TARE)** (by Science and Engineering Research Board)  
2 Sept 2021 to 10 Sept 2022 **Student Research Program** (by Pandit Deendayal Energy University)

## Memberships

Member of Royal Society of Chemistry (MRSC): 719271  
Indian Society of Chemists and Biologists (ISCB): 1161/2022  
International Society for Computational Biology and Bioinformatics (ISCB): 37142  
Member of the Drug Discovery World community

## Journal Editor

Computational Biology and Bioinformatics ISSN: 2330-8281 (Online)  
Journal of Molecular Docking: ISSN: 2798-138X (online)

## Editorial Contributions

Editor (Frontiers in Tropical Diseases): In Silico Methods and Artificial Intelligence In Antimalarial Drug Discovery

## Journal Reviewer

Journal of Biomolecular structure and Dynamics ISSN: 1538-0254 (Online)  
Scientific Nature: ISSN: 1476-4687 (online)  
Materials Today: Proceedings ISSN: 2214-7853 (online)  
Letters in Drug Design & Discovery ISSN: 1875-628X (Online)  
Journal of Molecular Modeling ISSN: 0948-5023 (Online)

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## Education

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

## Research Experience

- Nov 2019 – Mar 2020* **DST-SERB Research Associate**  
School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India
- Jul 2019 – Nov 2019* **DST-SERB Senior Research Fellow**  
School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India
- Jul 2017 – Jul 2019* **DST-SERB Junior Research Fellow**  
School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India
- Jan 2016 – Feb 2020* **PhD Student**  
School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India
- Aug 2014 – Jan 2016* **M.Phil. Student**  
School of Chemical Sciences, Central University of Gujarat, Gandhinagar, Gujarat, India
- Aug 2012 – Jul 2013* **Master's Student**  
Department of Science and Technology, Lovely Professional University, Phagwara, Punjab, India

## Awards

- Sept 2022* Award: NPTEL-AICTE Elite online certification awarded for successful completion of 8-week FDP on the theme “Computer Aided Drug Design” with consolidate score of 72% conducted by NPTEL-AICTE, funded by MoE, Govt. of India
- Apr 2022* Award: Best Poster Presentation, Two days international e-conference on Recent advancements in Chemical Sciences: Health, Environment and Society (ICRACS-2022) organized by Department of Chemistry, Deshbandhu College, University of Delhi
- Feb 2020* Award: Best Oral Presentation, National Science Day, organized by School of Nano Sciences, Central University of Gujarat, India
- Jul 2019* Award: 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* Award: Best Poster Presentation, National Conference on Applied Materials Science, organized by Centre for Applied Chemistry, Central University of Gujarat, India
- Jul 2017* Award: 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* Award: 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* Award: Best Poster Presentation, International Conference on Drug Design, organized

by Schrodinger at Jawaharlal Nehru University, India

*Feb 2016* Award: Best Poster Presentation, National Science Day, organized by School of Chemical Sciences, Central University of Gujarat, India

*Mar 2015* Award: Cleared GATE exam

*Aug 2013* Award: M.Sc. (Hons.) Chemistry Batch Topper

## Dissertation/Thesis Advisor

*B.Sc.* Guided four B.Sc. students for their bachelor-level project

*M.Sc.* Guided two M.Sc. students in their one-year research project funded by PDEU

*Ph.D.* One student is pursuing Ph.D.

## Skills and Expertise

*Skills* 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)

### *Expertise*

*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

## Journal Publications

*Total Publications: 30 (including book chapters, and proceedings)*

1. Soni, Jay, Nusrat Sahiba, Ayushi Sethiya, Pankaj Teli, Dinesh Kr Agarwal, **Anu Manhas**, Prakash Chandra Jha, Deepkumar Joshi, and Shikha Agarwal, *Polycyclic Aromatic Compounds* 2022, 42 (6), 2970–2990, DOI: 10.1080/10406638.2020.1852277
2. Madhu Pandey, Divya Jadav, **Anu Manhas**, Siddhi Kediya, Nao Tsunoji, Rajesh Kumar, Sourav Das, Mahuya Bandyopadhyay, *Molecular Catalysis* 2022, 525, 112365, DOI:10.1016/j.mcat.2022.112365
3. **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**)
4. Amar Ghosh, **Anu Manhas\***, Prakash C. Jha, *Journal of Cellular Biochemistry* 2022, 123, 628-643, DOI: 10.1002/jcb.30209 (**\*Corresponding Author**)
5. 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

6. Siddhi Kediya, **Anu Manhas**, Prakash C. Jha, *Journal of Physical Organic Chemistry* 2022, 35(1), e4283, DOI:10.1002/poc.4283
7. 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
8. Kediya, Siddhiben\*, **Anu Manhas\***, Mohsin Y. Lone, and Prakash C. Jha, *Journal of Molecular Structure* 2020, 1228, 129443, DOI:10.1016/j.molstruc.2020.129443 (\***Equal Contribution**)
9. **Anu Manhas\***, Sujeet Kumar, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2022, 40(1), 31-43, DOI:10.1080/07391102.2020.1806110 (\***Corresponding Author**)
10. 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
11. 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
12. Nusrat Sahiba, Dinesh K. Agarwal, **Anu Manhas**, Ayushi Sethiya, Jay Soni, Prakash C. Jha & Shikha Agarwal, *Polycyclic Aromatic Compounds* 2022, 42(4), 1201-1219, DOI:10.1080/10406638.2020.1768565
13. Siddhi Kediya, **Anu Manhas**, Prakash C. Jha, *ChemistrySelect* 2020, 5(18), 5437-5450, DOI:10.1002/slct.202000550
14. **Anu Manhas**, Saikat Dubey, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2020, 38(9), 2704-2716, DOI:10.1080/07391102.2019.1644197
15. **Anu Manhas**, Dhaval Patel, Mohsin Y. Lone, Prakash C. Jha, *Journal of Cellular Biochemistry* 2019, 120(9), 14531-14543, DOI:10.1002/jcb.28714
16. **Anu Manhas**, Mohsin Y. Lone, Prakash C. Jha, *Journal of Biomolecular Structure & Dynamics* 2019, 37(16), 4181-4199, DOI:10.1080/07391102.2018.1540362
17. **Anu Manhas**, Mohsin Y. Lone, Prakash C. Jha, *Molecular Diversity* 2019, 23(2), 453-470, DOI:10.1007/s11030-018-9885-5
18. **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
19. 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
20. 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
21. 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
22. **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
23. **Anu Manhas**, Sivakumar P. Kumar, Prakash C. Jha, *RSC Advances* 2016, 6 (35), 29466-29485, DOI:10.1039/C6RA01071G

24. Vijay Kumar, Niraj Upadhyay, **Anu Manhas**, *Journal of Molecular Structure* 2015, 1099, 135-141, DOI:10.1016/j.molstruc.2015.06.055
25. 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

### Proceeding Publications

1. Megha Balha\*, Nikunj Kumar Vagadiya, **Anu Manhas\*** *Materials Today: Proceedings* 2022, 62(13), 7007-7018, DOI: 10.1016/j.matpr.2021.12.546 (**\*Corresponding Author**)
2. **Anu Manhas\***, Mohsin Yousuf Lone, Prakash Chandra Jha *Materials Today: Proceedings* 2022, 62(13), 7109-7112, DOI: 10.1016/j.matpr.2022.02.032 (**\*Corresponding Author**)

### Book Chapter Publications

1. Nikunj Kumar Vagadiya, Mohil Odedara, Aayushi Joshi, Manoj Pandey, **Anu Manhas\***, Nandini Mukherjee\* *Springer Proceedings in Materials* 2022, 15, 221–232, In: Mukherjee, K., Layek, R.K., De, D. (eds) Tailored Functional Materials. Springer Proceedings in Materials, Singapore. DOI: 10.1007/978-981-19-2572-6\_17 ISBN: 978-981-19-2572-6 (**\*Corresponding Author**)
2. Aayushi Joshi, Nikunj Kumar Vagadiya, Mohil Odedara, Manoj Pandey, **Anu Manhas\***, Nandini Mukherjee\* *Springer Proceedings in Materials* 2022, 15, 209–220, In: Mukherjee, K., Layek, R.K., De, D. (eds) Tailored Functional Materials. Springer Proceedings in Materials, Singapore. DOI: 10.1007/978-981-19-2572-6\_16 ISBN: 978-981-19-2572-6 (**\*Corresponding Author**)
3. **Anu Manhas\***, Siddhi Kediya, Prakash Chandra Jha *Frontiers in Computational Chemistry* 2022, 6, Chapter 4, 132-192, Zaheer Ul-Haq, Angila K Wilson (eds) Bentham Book, Chapter DOI: 10.2174/9789815036848122060006, Book DOI: 10.2174/9789815036 8481220601, eISBN: 978-981-5036-84-8, 2022, ISBN: 978-981-5036-85-5, ISSN: 2352-944X (Print), ISSN: 2352-9458 (Online) (**\*Corresponding Author**)

### Faculty Development Programme

1. 8-week FDP on the theme “Computer Aided Drug Design” conducted by NPTEL-AICTE, funded by MoE, Govt. of India (July to Sept, 2022)
2. 5-day online FDP on the theme “Inculcating Universal Human Values in Technical Education” organized by All India Council for Technical Education (AICTE) from 11th July, 2022 to 15<sup>th</sup> July, 2022
3. 5-day online FDP on the theme “Inculcating Universal Human Values in Technical Education” organized by All India Council for Technical Education (AICTE) from 27th December, 2021 to 31st December, 2021

### Invited Speaker/Lecture Delivered

1. Delivered talk in Career Counselling by alumni in Central University of Gujarat (June 4, 2022)
2. Deliver lecture in Short-term course: Research interests in Pure and Applied Sciences organized by Sabarmati University (November 15-19, 2021)
3. Deliver lectures on Computer-aided drug designing at Central University of Gujarat (October 12-13, 2021)
4. Guest of Honor and Speaker in the 2nd International Conference on Recent Trends in Computational Cancer Biology and COVID-19 (ICRTCCBC-2021) (July 24-25, 2021) organized by BIOSHACK INDIA

## Organizer

1. Coordinated special session on Career Fair for UG/PG/PhD students in International Symposium on Materials of the Millennium: Emerging Trends and Future Prospects (MMETFP-2021) on 20 Nov, 2021
2. Four webinar series on “Multifarious Applications of Chemical Sciences” on 3<sup>rd</sup>, 10<sup>th</sup>, 17<sup>th</sup>, and 24<sup>th</sup> July, 2021
3. Webinar session on “Current and Emerging Career Opportunities in Chemistry” on 5<sup>th</sup> June, 2021
4. Webinar session on “2 Day International Webinar WASTE TO BEST: Sustainable Environmental Remediation Strategies & Solution” on 12<sup>th</sup> to 13<sup>th</sup> April, 2021
5. Webinar session on “THE SHE OF SCIENCE WORLD” on 8th March, 2021

## Conferences/Workshops Attended

### *International Conferences*

1. International conference on Drug Design: ICDD held at BITS, Goa India (10-11 November, 2022): Poster Presentation
2. Two days international e-conference on "Recent advancements in Chemical Sciences: Health, Environment and Society (ICRACS-2022) organized by Department of Chemistry, Deshbandhu College, University of Delhi (8-9 April, 2022): Poster Presentation
3. 1st International Conference on Advances in Water Treatment and Management held at Pandit Deendayal Energy University, Gandhinagar, Gujarat, India (25-26 March, 2022): Poster Presentation
4. 1st International Symposium on Materials of the Millennium: Emerging Trends and Future Prospects held at Pandit Deendayal Energy University, Gandhinagar, Gujarat, India (19-21 November, 2021): Attended
5. 1st International Conference on Additive Manufacturing and Advanced Materials (AM2) held at Pandit Deendayal Energy University, Gandhinagar, Gujarat, India (4-6 October, 2021): Oral Presentation
6. International Conference on Integrating Chemical, Biological, and Pharmaceutical Sciences for Innovation in Health Care by Indian Society of Chemists and Biologists held at Nirma University, India (22-24 January, 2020): Oral Presentation
7. International conference on Advanced Materials Science and Technology: ICAMST held at Bannari Amman Institute of Technology, Sathyamangalam, Tamil Nadu, India (17-19 August 2017): Poster Presentation
8. International conference on Frontiers at the Chemistry-Allied Sciences Interface held at University of Rajasthan, Jaipur, India (22-23 July, 2017): Oral Presentation
9. International conference on Drug Design: ICDD held at JNU Convention Centre, Jawaharlal Nehru University, New Delhi, India (07-09 April, 2017): Poster Presentation

### *National Conferences*

1. DAE symposium on Current Trend in Theoretical Chemistry Organized by Chemistry Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085, INDIA: Poster Presentation (Online)
2. National conference on Applied Materials Science held at Central University of Gujarat, India (6-7 April 2018): Poster Presentation



3. National conference on Challenges in Energy Conversion and Environmental Applications held at Bannari Amman Institute of Technology, Sathyamangalam, Tamil Nadu, India (23-24 March 2018): Poster Presentation
4. National conference on Nanotechnology in Agriculture, Energy and Medicine held at Central University of Gujarat, Gandhinagar, India (11-12 March, 2016): Attended
5. National conference on the Frontiers of Chemical Sciences and Potential Interfaces held at Central University of Gujarat, Gandhinagar, India (10-11 April, 2015): Attended
6. National conference on Science for Global Development, 3rd Bhartiya Vigyan Sammelan and Expo, held at Lovely Professional University, Punjab, India (11-14 October, 2012): Poster Presentation

### *Workshops*

1. Workshop on Advanced Simulation Methods: DFT, MD and Beyond held at Indian Institute of Technology Delhi, New Delhi, India (6-10 March, 2019)
2. Workshop on Free Energy Calculations For Chemical And Biological Systems held at Indian Institute of Technology Kanpur, UP, India (17-22 March, 2019)
3. Workshop on “Hands-on Practice on LaTeX” held at Sardar Vallabhbhai National Institute of Technology, Surat, India (07-09 October, 2016)
4. Workshop on Nuclear Magnetic Resonance Spectroscopy held at Saurashtra University, Rajkot (11-12 September, 2015)
5. Workshop on IPR (Patent) & Innovation held at Central University of Gujarat, Gandhinagar, India (14 August, 2015)
6. Workshop on Open Educational Resource held at Central University of Gujarat, Gandhinagar, India (25 July, 2015)

### *Webinars/Online Workshops Attended*

#### *International Webinars*

1. International virtual conference on Computer-Aided Drug Design organized by Department of Pharmacy, BITS Pilani, Pilani campus, India (30-31 October, 2020): Attended (Online)
2. International Virtual Conference on Frontiers in Chemical Sciences organized by Department of Chemistry, MLSU, Udaipur, Rajasthan, India (25 June, 2021): Attended (Online)

#### *National Webinars*

1. Webinar on Electrochemical Methods: Techniques to Application by Department of Chemistry, Pandit Deendayal Energy University, Gujarat, India (05 April, 2021): Attended (Online)
2. Webinar on AMAZING EARTH: SPACE TO SURFACE by Department of Physics, Chemistry and Mathematics, Pandit Deendayal Energy University, Gujarat, India (22 May, 2021): Attended (Online)

### *Workshops*

1. International online workshop on ARTIFICIAL INTELLIGENCE TOOLS FOR ACCELERATED DRUG DISCOVERY AGAINST COVID-19 by Department of Biotechnology, Vignan’s Foundation for Science,

Technology & Research, Vadlamudi-522213, Guntur, Andhra Pradesh, India (10-14 August, 2020):  
Attended (Online)

2. International E-workshop on Machine Learning applications in Drug Discovery: Basic to Advanced by Department of Biotechnology, Vignan's Foundation for Science, Technology & Research, Vadlamudi-522213, Guntur, Andhra Pradesh, India (17-31 May, 2021) (Online)

### Extra Responsibilities

1. Question paper setter: Nominated by the Registrar, Sabarmati University, Ahmedabad to be appointed as Question paper setter for Analytical Chemistry (2021, 2022)
2. External examiner appointment: Nominated by the Head of Department of Chemistry, Sabarmati University, Ahmedabad to be appointed as external examiner of Practical Viva Voce examination of M.Sc. Semester-I (2021, 2022)
3. Chemistry website coordinator (<https://sot.pdpu.ac.in/Chemistry-dept.html>): Nominated by the Head of Department of Chemistry, Pandit Deendayal Energy University
4. Chemistry Newsletter coordinator (Chemstreet): Nominated by the Head of Department of Chemistry, Pandit Deendayal Energy University
5. Course file Coordinator: Nominated by the Head of Department, Chemistry, Pandit Deendayal Energy University
6. Actively involved in the admissions process (University Services): Nominated by the Director of School of Technology, Pandit Deendayal Energy University
7. Contributed in designing the CURRICULUM of
  - MSc Theoretical & Computational Chemistry PDEU (2020-2022, 2021-2023)
  - MSc Theoretical & Computational Chemistry Practical PDEU (2020-2022, 2021-2023)
  - BSc Quantum & Computational Chemistry (2022-2023)
  - PhD Computational Chemistry (2021-2022)
  - PhD Structural Bioinformatics (2021-2022)

### Extracurricular Activities Awards

2021-2022 First position in PDBL (Pandit Deendayal Badminton League)  
2018-2019 First position in carom mix doubles match  
Second position in badminton singles match  
Second position in badminton mix doubles match  
2017-2018 Third position in Quiz  
2016-2017 First position in carom singles match  
2015-2016 Third position in Kho-Kho women's match  
2014-2015 Second position in street play  
Third position in Kho-Kho women's match  
Third position in Cricket women's match



## Personal Details

<i>Name</i>	Anu Manhas	<i>Nationality</i>	Indian
<i>Father's Name</i>	Rishi Kumar	<i>Sex</i>	Female
<i>Mother's Name</i>	Nirmal Kumari	<i>Marital Status</i>	Single
<i>Date of Birth</i>	01-03-1991	<i>Language</i>	English, Hindi, Punjabi

## Declaration

I hereby declare that the details mentioned above are correct to the best of my knowledge and belief. I bear the accountability for any error or mistake in the data if occurs in the future.

Name: Dr. Anu Manhas

Date: 25-11-2022