

CURRICULUM VITAE

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RESEARCH INTERESTS:

- X-RAY CRYSTALLOGRAPHY
- MOLECULAR MODELLING
- QUANTUM MECHANICAL CALCULATIONS

SUMMARY:

- Expertise in Protein expression, purification, crystallization, crystal mounting, data collection and structure solution
- Expertise in Crystallization of small molecules, mounting of crystal on the Goniometer Head of P4 single crystal X-Ray Diffractometer, Data collection and structure solution.
- Applied DFT based methods for the prediction of various electronic properties and conformation of molecules in vacuum. The comparison of different methods for optimization and estimation of intramolecular aromatic π - π interaction energies have been carried out.
- Docking studies of small molecules with targets, and ADME calculations in order to understand rational drug design.
- Molecular Dynamics simulation of Biomolecules and docked complexes.
- Good knowledge and working experience on crystallographic software like; COLLECT, HKL, MOSFILM, CCP4, PHENIX, XSCANS, SHELXTL-NT, WINGX, PLATON, MERCURY, ORTEP-3; computational chemistry software like GAUSSIAN, AMPAC and CALCUL; Molecular docking software AUTODOCK, GLIDE and Molecular Dynamics software DESMOND.

EDUCATION:

- Post-Doctoral Fellow at Albert Einstein College of Medicine, Bronx, New York, USA (2014-2015).
- Ph.D. (Physics) from *Deen Dayal Upadhyaya Gorakhpur University, Gorakhpur (U.P.), INDIA* awarded in January, 2010. Thesis title “*Crystallographic and Theoretical Studies on Some Aromatic Compounds of Biological Significance*”
- Qualified the *National Eligibility Test* organized by CSIR, New Delhi, INDIA in the year 1999 (June and December both) for Lectureship.
- M. Sc. (Physics) from *Deen Dayal Upadhyay Gorakhpur University, Gorakhpur (U.P.), INDIA* in 1999 with *First* Division
- B. Sc. (Physics, Mathematics and Chemistry) from *National P.G. College, Barhalganj, Gorakhpur (U.P.), INDIA* in 1997 with *First* Division
- Intermediate (Math group) from DAV Inter college, Mau in 1994 with first division
- High School (Science Group) from Govt. Jubilee Inter College, Gorakhpur with first division

TEACHING AND RESEARCH EXPERIENCE:

- **Post-Doctoral Research Fellow** at Albert Einstein College of Medicine, Bronx, New York, USA (24.09.2014 - 23.09.2015).
- **Professor:** Dept. of Physics, DDU Gorakhpur University, Gorakhpur (7th March 2016 to till date)
- **Associate Professor:** Dept. of Physics, DDU Gorakhpur University, Gorakhpur (7th March 2013 to 6th March, 2016)

- **Assistant Professor/Reader:** Department of Physics, DDU Gorakhpur University (20th Sept. 2003 to 6th March 2013)
- **Lecturer :** Department of Physics, MGPG College, Gorakhpur (March 7, 2001 to Sept 19, 2003)
- **JRF:** MSB Division, CDRI, Lucknow, INDIA (March 2000 to Feb. 2001)
- **JRF:** Dept. of Physics, BHU Varanasi (January 2000 to March 2000)

INVITED TALKS:

1. **“Protein-ligand docking using AUTODOCK”** in the **workshop** on *“Computational methods in Physical, Geological Modeling and Drug Designing”* held during 29th September to 1st October 2011, organized jointly by National Centre of Experimental Mineralogy and Petrology(NCEMP), University of Allahabad and National Academy of Sciences, India(NASI), Allahabad Chapter.
2. **“X-Ray Crystallographic Investigations and docking studies with viper Phospholipase A2 on Some dissymmetrical Leonard linker pyrazolo[3,4-*d*]pyrimidine compounds and MD simulation of the best docked poses”** at the 42nd *National Seminar on Crystallography(NSC42)* held during November 21-23, 2013 organized by JNU, New Delhi.
3. **“Structural and Functional Characterizations of Solute binding Proteins by Differential Scanning Fluorimetry and Crystallography”**. American Crystallographic Association Meeting 2015, Philadelphia, PA, USA from July 25 to 29, 2015.
4. **“Discovery of cognate ligands for Solute Binding Proteins utilizing DSF and Crystallography”** during *National conference on “Climate change, Medicinal Plants and Public Health: Strategizing an ethanobotanical-social resilience”* during Jan 27-28, 2016 organized by Department of Botany, St. Andrews College, Gorakhpur.
5. **“Structural and Functional Characterizations of SBPs by Differential Scanning Fluorimetry and Crystallography”** at *“National Seminar on Nano Science and Nanobiotechnology”* held during February 25-26, 2017 at Department of Physics, DAV College, Kanpur
6. **“DSF Screening and X-Ray Crystallographic Investigations on Solute Binding Proteins”**, at 45th *National Seminar on Crystallography(NSC45)* held during July 9-12, 2017 at IIT BHU, Varanasi
7. **“Nuclear Decay”**, during Workshop on *Recent Trends in Physical Sciences*, organized by M.G.P.G. College, Gorakhpur during April 12-16, 2018.
8. **“Solute Binding Proteins: Structure, Function and their role in functional annotation”** at 22nd *International Conference of International Academy of Physical Sciences on Emerging trends in Physical Sciences* during April 13-15, 2018 organized by Faculty of Science, Dr. RML University Faizabad -224001, U.P., India.
9. **“Structure, Function, and Dynamics of Solute Binding Proteins”** at *National Seminar on Biotechnological Intervention in Agriculture, Health and Industry* during 23-24 Feb 2019 organized by Department of Biotechnology, DDU Gorakhpur University, Gorakhpur.
10. **Structure, Function and Dynamics of Solute Binding Proteins** at National Seminar on Recent Advances in Material Science and Electronics (RAMSE-2019) during Feb 27-28, 2019 organized by Department of Physics and Electronics, Dr. Ram Manohar Lohia Avadh University, Ayodhya.
11. **“Solute Binding Proteins as Smart Biomolecules: Structural and Functional Characterizations”** at *National Conference on Smart Materials, Devices and Sustainable Technologies* during 15-16 March 2019 organised by the Department of Applied Physics, MMM University of Technology, Gorakhpur
12. **“Solute Binding Proteins and their cognate ligands: Structure, Function and their role in functional annotation”** at *International Conference on Advanced Spectroscopy, Crystallography and Applications in Modern Chemistry* during April 25-26, 2019 at Rome, Italy.
13. **“An Introduction to Biomolecular Simulation and Drug Design”** at National workshop on Modeling and Simulation of microstrip antenna , circuits and materials organized by Department of Physics and Electronics, Dr RML Awadh University, Ayodhya during Jan 27- Feb 2, 2020.

14. **“Solute binding proteins as smart biomolecules: structural and functional characterizations”** at International conference on frontier areas of chemistry (ICFAC2020) organized by School of Physical Sciences, Mahatma Gandhi Central University, Motihari, Bihar during Feb 28-29, 2020.
15. **“Structure based drug discovery of tubulin binding agents from botanical extracts having potential anticancer properties”** at the National Conference on “Traditional medicine systems: their relevance and importance in health care systems of today and tomorrow” held on July 2-3, 2020 at St. Andrews College Gorakhpur.
16. **“Structure-based drug discovery of Natural Products as SARS-CoV-2 Mpro Antagonist from Echinacea angustifolia”** at the National Conference on “Traditional medicine and Ethnobotany: Exploring New horizons in Traditional and Alternative Medicine” held on July 19-20, 2021 at St. Andrews’ College, Gorakhpur.
17. **“Computational Tools and Methods for Drug Discovery”**, during National workshop on “Research Methodology & Innovations in Life Sciences” organized by Department of Biotechnology, DDU Gorakhpur University, from 25th June-1st July, 2021.
18. **“Biophysical methods in drug discovery”** during *IMPACT Lecture Series* on October 7-8, 2021 at St. Andrews College, Gorakhpur Sponsored by **Institutions Innovation Council**, Ministry of Education, New Delhi.
19. **“Physical Aspects of Biomolecular Simulations and Drug Design”** during National workshop on “Research Methodologies for Multidisciplinary Perspectives of Physics” organized by Department of Physics, DDU Gorakhpur University, Gorakhpur during June 29 – July 5, 2021.
20. **“Quantum mechanics and its applications”**, an expert lecture under MPHEQIP program at Govt. Sanjay Gandhi PG College, Ganj Basoda, Vidisha, M.P. 14.11.2022
21. **“Structure-based drug discovery of Natural Products as SARS-CoV-2 Mpro Antagonist from Echinacea angustifolia”**, at National Seminar on Recent Trends in Multifunctional Materials, organized by Department of Physics, M.L.K. PG College, Balrampur during 17-18 December 2022.
22. **“Structure based Investigation of natural compounds as SARS-CoV-2 Mpro antagonists”** at the International Conference of Advancements in Functional Materials (ICAFM-2024) organized by Rajju Bhैया Institute of Physical Sciences for study and research, VBS Poorvanchal University, Jaunpur during Feb 8 – 10 , 2024.

Chairman/co-chairman during technical sessions in Conferences/Seminars/Symposia/workshops

- **Session Co-chairman:** National workshop on “*Scientific paper writing and effective communication*” during Sept 17-18, 2016 organized by Department of Biotechnology, DDU Gorakhpur University, Gorakhpur
- **Session Chairman:** National Seminar on *Nanoscience and Nanobiotechnology* held during February 25-26, 2017 at Department of Physics, DAV College, Kanpur
- **Session Chairman:** 22nd International Conference of *International Academy of Physical Sciences on Emerging trends in Physical Sciences* during April 13-15, 2018 organized by Faculty of Science, Dr. RML University Faizabad -224001, U.P., India
- **Session Chairman:** *National Conference on Smart Materials, Devices and Sustainable Technologies* during 15-16 March 2019 organised by the Department of Applied Physics, MMM University of Technology, Gorakhpur
- **Session Chairman:** National Conference on Omics for Food, Health and Environment (OFHE-2020) organized by Department of Biotechnology, DDU Gorakhpur University, Gorakhpur
- **Session Chairman:** 5th International Conference on Microelectronics, Computing & Communication Systems (MCCS-2020) organized by IETE & ISVE at Advanced Regional Telecom Training Centre, BSNL, Hazaribag Road, Ranchi- 835217, Jharkhand, India during July 11-12,2020.
- **Session Chairman:** 6th International Conference on Nanoelectronics Circuits & Communication Systems (NCCS-2020) organized by IETE & ISVE at Advanced Regional Telecom Training Centre, BSNL, Hazaribag Road, Ranchi- 835217, Jharkhand, India during Dec 19 -20, 2020.

- **Session Chairman:** International conference on Futuristic materials (ICFM20) organized by Department of Physics, DDU Gorakhpur University, Gorakhpur during 18-20 Dec, 2020.
- **Session Chairman:** 7th International Conference on Microelectronics, Computing & Communication Systems (MCCS-2022) on 9-10th July 2022 at ARTTC, BSNL near Jumar River, Hazaribag Road, Ranchi
- **Session Chairman :** National Seminar on Recent Trends in Multifunctional Materials, organized by Department of Physics, M.L.K. PG College, Balrampur during 17-18 December 2022

PROJECTS UNDERTAKEN:

- UGC Minor research project entitled “*Study of Structure and conformation of some biomolecules using crystallographic and theoretical techniques*” (no. F 31-32/2005 (SR)), Amount mobilized: Rs. 50,000/-, duration: 1st April 2006 to 31st March 2008.
- Worked on the project “*Grand canonical ensemble simulation of adsorption in zeolites*” during May 8 –July 2, 2011 at Solid State and Structural Chemistry Unit, IISc, Bangalore under the supervision of Prof. S. Yashonath under summer research fellowship program funded jointly by the three Science Academies of India (IASc, Bangalore; INSA, New Delhi; NASI, Allahabad)
- DST Fast Track Project entitled “*Synthesis ,X-ray crystallographic and computational studies on some pyrazolo[3,4-d] pyrimidines*” (Ref. No.-SR/FT/CS-78/2010), Amount mobilized Rs. 21.80 Lakh, duration: 07 March, 2011 to 06 March 2014.
- UGC's Raman Fellowship award to work on "*Structural Genomics of Anaerobic pathogens*" (F.No. 55-1/2013(IC)), Amount mobilized: Rs.23,22,548/-, duration: 24th September, 2014 to 23rd September 2015.
- CST UP sponsored major research project entitled “Investigations of novel tubulin binding agents with potential anticancer properties using various computational techniques” (Ref. no. CST/D-1526), amount mobilized : Rs. 11,86,000/- duration: 04-01-2024 to 03-01-2027

FELLOWSHIPS/AWARDS:

- **International Travel Award by CSIR, New Delhi to deliver an Invited Talk during the "International Conference on Advanced Spectroscopy, Crystallography and Applications in Modern Chemistry"** during April 25-26, 2019 at Rome, Italy.
- **Raman Fellowship** for Post-doctoral Studies in USA for the year 2014-2015 awarded by UGC, New Delhi, India(2014).
- **Young Scientist**, awarded by DST, New Delhi under DST FAST-Track Young Scientist Scheme (2011).
- **Summer Research Fellowship** awarded jointly by IASc, Bangalore; INSA, New Delhi; NASI, Allahabad(2011).

SYMPOSIUM/SEMINAR ORGANISED:

- Organizing Secretary “National Symposium on Advanced Materials Science” during 7 & 8 December 2018 at the Department of Physics, DDU Gorakhpur University, Gorakhpur: organizing Secretary
- Coordinator, Water Sector of the “National webinar cum seminar on Sustainable development of Poorvanchal: Issues, strategies and a way forward” held on December 10-12, 2020 organised by DDU Gorakhpur University and Planning department, Govt of Uttar Pradesh.
- Coordinator, 6th Interdisciplinary Refresher Course on “Information Communication Technology” organized by UGC-HRDC, DDU Gorakhpur University during Sept. 27 to Oct. 10, 2021
- Coordinator, 7th Interdisciplinary Refresher Course on “Information Communication Technology” organized by UGC-HRDC, DDU Gorakhpur University during Jan. 28 to Feb. 10, 2023.

ADMINISTRATIVE EXPERIENCE:

- Director, Institute of Engineering and Technology, DDU Gorakhpur University, Gorakhpur (22nd November 2023 to till date)
- Warden, Sant Kabir Hostel, DDU Gorakhpur University, Gorakhpur (15th June 2021 to till date)
- Program Officer, NSS (Shastri Unit), DDU Gorakhpur University (From 2012-13 to 2013-2014)
- Assistant Proctor at DDU Gorakhpur University, Gorakhpur (2005-2006)
- Assistant Proctor at MGPG College, Gorakhpur (2002-2003)
- Sports Team manager: MGPG College, Gorakhpur (2002-2003)

LIFE MEMBERSHIPS:

- Indian Crystallographic Association
- Indian Biophysical Society
- Indian Association of Physics Teachers
- American Crystallographic Association
- Indian Science Congress Association (L31014)

Orientation/Refresher Courses attended

- 50th orientation course held at ASC, DDU Gorakhpur University (Jan 2- 31, 2003)
- P.G. level Refresher course in Physics held at I.M.Sc., Chennai (May 26 - June 15, 2005).
- IIIrd Refresher course in Physics held at the Dept. of Physics, DDU Gorakhpur University (Sept 7- 27, 2007).
- IVth Refresher course in Physics held at the Dept. of Physics, DDU Gorakhpur University, (December 11-31, 2009).
- IVth Refresher Course in Environmental Science held at the Dept. of Zoology, DDU Gorakhpur University (Sept 29 - Oct 19, 2012).
- Vth Refresher course in the Department of Physics, DDU Gorakhpur University, Gorakhpur (Feb 11, 2014 to March 3, 2014)
- VIIth refresher course in "Environmental Studies(ID): "Man and Biosphere" held at Human resource development center, DDU Gorakhpur University, Gorakhpur (Nov 18- Dec 8, 2015)

Ph.D. Supervised:

1. Bindesh Kumar Shukla, Thesis title: Modeling Studies on some molecules of biological significance, awarded on September, 2016.
2. Hari Om Gupta, Thesis Title: Computational studies on the structure and dynamics of some bioactive molecules, August 2017.
3. Sanjai Kumar Yadav, Thesis Title: Modeling studies on DNA minor groove binders, January 2020.

Guest Associate Editor:

1. Frontiers in Molecular Biosciences, Volume 9, 2022, section: Molecular Diagnostics and Therapeutics; Impact factor : 6.1
2. Molecules, (in progress), MDPI publications; Impact factor : 4.9

LIST OF PUBLICATIONS

(I) Books:

1. *X-ray Crystallographic and Theoretical Investigations on Aromatic Compounds*. Umesh Yadava and Mihir Roychaudhary, ISBN: 978-3-8443-0404-6, LAP Lambert Academic Publishing GMBH and Co. KG, Dudweiler Landstr. 99, 66123, Saarbrücken, Germany. 2011
2. *Effect of Heat Processing on the Vitamin-C of Some Fruits*. Seema Gudden and Umesh Yadava, ISBN: 978-3-6591-1924-8, LAP Lambert Academic Publishing GMBH and Co. KG, Dudweiler Landstr. 99, 66123, Saarbrücken, Germany. 2011

3. *Synthesis, Characterization and application of Mn(III) complex compounds*. Seema gudden, Sudha Yadava and **Umesh Yadava**. ISBN: 978-3-6591-3004-5. LAP Lambert Academic Publishing GMBH and Co. KG, Dudweiler Landstr. 99, 66123, Saarbrücken, Germany. 2012
4. *Investigations on medicinal attributes of pyrazolo[3,4-d]pyrimidines*. **Umesh Yadava**, Maheshwer Singh and Mihir Roychoudhury. ISBN-13: 978-36596-2262-5. LAP Lambert Academic Publishing GMBH and Co. KG, Dudweiler Landstr. 99, 66123, Saarbrücken, Germany. 2016
5. *Molecular Modeling Investigations on Pyrazolo[3,4-d]pyrimidines*, Bindesh Kumar Shukla and Umesh Yadava, ISBN: 978-6202075473, . LAP Lambert Academic Publishing GMBH and Co. KG, Dudweiler Landstr. 99, 66123, Saarbrücken, Germany, 2019
6. *A Text Book of Mechanics*, R.B. Singh, **Umesh Yadava**, A.K. Dwivedi, S.A. Khan, Kanha Publishing House, Gorakhpur. ISBN: 978-81-932123-3-2
7. *A Text Book of Electricity and Magnetism*, R.B. Singh, **Umesh Yadava**, J.P. Pandey, V.P. Srivastava, Indrajeet Mishra, U.S.P. Yadav, Kanha Publishing House, Gorakhpur. ISBN: 978-81-932123-4-9

Chapter:

1. **Single Crystal X-ray structure Determination:** in “*Theoretical and computational advances: from atoms to molecules to materials*” ISBN: 978-93-5196-507-7 published by **Self Publishing, Lucknow (U. P.) INDIA**, 2017

(II) Published Research Articles-

1. Guggulsterone E, a lipid-lowering agent from Commiphora mukul, S. Sarkhel, **Umesh Yadava**, P. Prakas, G. K. Jain, S. Singh and P. R. Maulik, *Acta Cryst.* (2001) **E57**, o285-o286. (Impact Factor: 0.8)
2. A taxane diterpenoid from the needles of Taxus Wallichiana, S.K. Chattopadhyay, A. Sharon, **Umesh Yadava**, S. Srivastava, V.K. Mehta and P.R. Maulik, *Acta Cryst.* (2001) **E57**, o1158-o1160. (IF: 0.8)
3. A taxane diterpenoid from the heartwood of Taxus Wallichiana, S.K. Chatopadhyay, A. Sharon, **Umesh Yadava**, S. Srivastava, V.K. Mehta and P. R. Maulik, *Acta Cryst.* (2002) **E58**, o154-o155. (IF: 0.8)
4. Unusual molecular conformation in dissymmetric propylene linker compounds containing pyrazolo[3,4-d]pyrimidine and phthalimide moieties, K. Avasthi, D. Bhagat, C. Bal, A. Sharon, **Umesh Yadava** and P. R. Maulik, *Acta Cryst.* (2003) **C59**, o409-o412. (IF: 8.3)
5. Facile synthesis of 2-arylbenzo[b]furans through unusual acid catalysed 1,2-elimination, A. K. Jha, P. C. Sharma, P. R. Maulik, **Umesh Yadava** & K. Hajela, *Ind. J. Chem.* (2004) **43B**, 1341-1344. (IF: 0.6)
6. Fine tuning of folded conformation by change of substituents : ¹H NMR and crystallographic evidence for folded conformation due to arene interactions in pyrazolo[3,4-d]pyrimidine core based ‘propylene linker compounds’, K. Avasthi, S. Aswal, R. Kumar, **Umesh Yadava**, D. S. Rawat and P. R. Maulik, *J. Mol. Struct.* (2005) **750**, 179-185. (IF: 1.4)
7. 5,8-diethyl-6,9-dithioxo-2,3,5,6,8,9-hexahydro-1H-3a,5,8,9a-tetraazaphenalene-4,7-dione, **Umesh Yadava**, Atul Goel, V. J. Ram and P. R. Maulik., *Acta Cryst.* (2006) **E62**, o4991-o4993. (IF: 0.8)
8. Crystal structure analysis of (2,3-dihydro-3-hydroxy-2-phenylbenzo[b]furan-2-yl)(4-methoxyphenyl)methanone , **Umesh Yadava***, M. Roychoudhury and P. R. Maulik, *J. Curr. Sci.* (2008) **12(2)**,723-728.
9. Theoretical investigations on molecular structure and IR frequencies of 4-n-nonyl-4'-cyanobiphenyl in light of experimental results, **Umesh Yadava***, Dinesh K. Gupta and Mihir Roychoudhury, *J. Mol. Liq.* (2010) **156**, 187-190. (IF: 4.5)
10. Gas-phase conformational and intramolecular π - π interaction studies on some pyrazolo[3,4-d]pyrimidine derivatives, **Umesh Yadava***, Maheshwer Singh, Mihir Roychoudhury, *Comput. Theor. Chem.* (2011) **977**, 134-139. (IF: 1.5)
11. A comparison of crystallographic and DFT optimized geometries on two taxane diterpenoids and docking studies with phospholipase A2, **Umesh Yadava***, Hariom Gupta & Mihir Roychoudhury, *Med. Chem. Res.* (2012) **21(9)**, 2162-2168. (IF: 1.3)
12. 2,2'-Bipyridyl-acetylphenolato mixed ligand copper(II) complexes: Syntheses, characterizations and catalytic activity in styrene epoxidation, Shyamapada Shit, **Umesh Yadava**, Debraj Saha, Roland Frohlich, *J. Coord. Chem.* (2013) **66(1)**, 66-76. (IF: 2.23)

13. Pyrazolo[3,4-d]pyrimidines as inhibitor of anti-coagulation and inflammation activities of phospholipase A2 : insight from molecular docking studies, **Umesh Yadava***, Maheshwer Singh & Mihir Roychoudhury, *J. Biol. Phys.* (2013) **39**, 419-438. (IF: 1.6)
14. Molecular dynamics simulation of DNA duplex, analog of PPT (polypurine tract), its conformation and hydration: a theoretical study. Ramesh Kumar Yadav & **Umesh Yadava***, *Med. Chem. Res.* (2014) **23**, 280-286. (IF: 1.3)
15. Synthesis, spectral characterization and antimicrobial studies of nano-sized oxovanadium(IV) complexes with Schiff bases derived from 5-(phenyl/substituted phenyl)-2-hydrazino-1,3,4-thiadiazole and indoline-2,3-dione, M.K. Sahani, **U. Yadava**, O.P. Pandey, S.K. Sengupta. *Spectrochimica Acta Part A: Mol. Biomol. Spect.* **125** (2014) 189–194. (IF: 2.5)
16. Determination of distances and sizes of visible objects using a plane transparent glass plate, Arvind Kumar Pandey and **Umesh Yadava***, *Results in Phys.* **4** (2014) 83-87. (IF: 1.2)
17. Molecular modeling and structural studies of 12-mer immobile four-way DNA junction in solution, Ramesh Kumar Yadav and **Umesh Yadava***, *Bioinformation* **10**(7) (2014) 86-97.
18. Docking and Molecular Dynamics Simulations of Pyrazolo[3,4-d]Pyrimidine-DNA Complexes, **Umesh Yadava**, Hariom Gupta, Ramesh Kumar Yadav, and Mihir Roychoudhury, *Advanced Science Letters*, **20**, 1637–1643, 2014. (IF: 1.2)
19. *In-Silico* Docking Studies of Some Pyrazolo [3,4-D]pyrimidine Derivatives: A Novel Inhibitor of Mycobacterium Tuberculosis, Bindesh Kumar Shukla and **Umesh Yadava**, *Int J Res Eng Biosc* 2(5) (2014) 48-56.
20. Stabilization of Microtubules by Taxane Diterpenoids: Insight from Docking and MD simulations, **Umesh Yadava**, Hariom Gupta & Mihir Roychoudhury, *J Biol Phys* (2015) 41:117–133. (IF: 1.6)
21. Synthesis, QSAR and anticandidal evaluation of 1,2,3-triazoles derived from naturally bioactive scaffolds, Mohammad Irfan, Babita Aneja, **Umesh Yadava**, Shabana I. Khan, Nikhat Manzoor, Constantin G. Daniliuc, Mohammad Abid. *Eur. J. Med. Chem.* **93** (2015) 246-254 (IF: 4.8)
22. Pyrazolo[3,4-d]pyrimidines as novel inhibitors of O-acetyl-L-serine sulfhydrylase of Entamoeba histolytica: an in silico study, **Umesh Yadava**, Bindesh Kumar Shukla, Mihir Roychoudhury, Devesh Kumar, *J Mol Model* (2015) **21**: 96 (IF: 1.8)
23. Diketo acids and their amino acid/dipeptidic analogues as promising scaffolds for the development of bacterial methionine aminopeptidase inhibitors, Mir Mohammad Masood, Vijay K. Pillalamarri, Mohammad Irfan, Babita Aneja, Mohamad Aman Jairajpuri, Md. Zafaryab, M. Moshahid A. Rizvi, **Umesh Yadava**, Anthony Addlagatta and Mohammad Abid. *RSC Adv.*, 2015, **5**, 34173-183 (IF: 3.2)
24. Pyrazolo[3,4-d]pyrimidines as the inhibitors of mycobacterial β -oxidation trifunctional enzyme, **Umesh Yadava**, Bindesh Kumar Shukla, Mihir Roychoudhury, *Med Chem Res*, **24** (2015) 4002-4015. (IF: 1.4)
25. Theoretical explorations on the molecular structure and IR frequencies of 3-phenyl-1-tosyl-1H-pyrazolo[3,4-d]pyrimidin-4-amine in view of experimental results, Bindesh Kumar Shukla, **Umesh Yadava**, Mihir Roychoudhury, *J. Mol. Liq.* **212** (2015) 325–330 (IF: 4.5)
26. An unusual conformational change in the folded trimethylene/Leonard linker pyrazolo[3,4-d]pyrimidine analogue of the theophylline compound due to structural changes, K. Avasthi, Ruchir Kant, S. Aswal, A. K. Tewari, **Umesh Yadava**, U. D. Misra and P. R. Maulik, *J. Struct. Chem.*, **56**(7) (2015) 1437-1440. (IF: 0.8)
27. Molecular dynamics simulation of microtubule and its inhibitor complexes: in silico search for anticancer drugs, **Umesh Yadava**, Hari Om Gupta and Ramesh Kumar Yadav, *Int J Res Eng Biosci* 3(5) (2015) 42-52.
28. Molecular dynamics simulation of hydrated d(CGCGTACCCG)₄ as a four-way DNA Holliday junction and comparison with the crystallographic structure, Ramesh Kumar Yadav and **Umesh Yadava**, *Molecular Simulation*, 2016, **42**, 25-30. (IF: 1.5)
29. Monocyclic β -lactam and unexpected oxazinone formation: synthesis, crystal structure, docking studies and antibacterial evaluation, Babita Aneja, Mohammad Irfan, Md. Imtaiyaz Hassan, Amresh Prakash, **Umesh Yadava**, Constantin G. Daniliuc, Md. Zafaryab, M. Moshahid A. Rizvi, Amir Azam, and Mohammad Abid, *J Enzyme Inhib Med Chem*, **31**(5) (2016) 834-852 DOI: 10.3109/14756366.2015.1058257 (IF: 4.5)
30. Synthesis and Crystal Structure Analysis of Monocyclic β -Lactam Derivatives, Alam S, Hasan P, Aneja B, Md Ahmad B, **Yadava U**, Daniliuc CG and Abid M, *Struct. Chem. Crystall. Comm.*, **2** (2016) 19

31. Structure of an ABC transporter solute-binding protein specific for the amino sugars glucosamine and galactosamine, **Umesh Yadava**, Matthew W. Vetting, Nawar Al Obaidi, Michael S. Carter, John A. Gerlt and Steven C. Almo, *Acta Cryst. F* **72** (2016), 467–472. (IF: 0.9)
32. QSAR Study of Some Pyrazolo[3,4-d]pyrimidine Derivatives as the c-Src Inhibitors, Bindesh Kumar Shukla and **Umesh Yadava**, *AIP Conf. Proceed* **1728** (2016) 020320: 1-4. DOI: 10.1063/1.4946371 (IF: 0.6)
33. Efficient synthesis of novel N-substituted 2- carboxy-4-quinolones via lithium bis(trimethylsilyl) amide (LiHMDS)-induced in situ cyclocondensation reaction, Phool Hasan, Babita Aneja, Mir M. Masood, Md. Belal Ahmad, **Umesh Yadava**, Constantin G. Daniliuc and Mohammad Abid, *RSC Adv.* **7** (2017) 11367-11372. (IF: 3.2)
34. Novel anti-tubulin agents from plant and marine origins: insight from a molecular modeling and dynamics study. **Umesh Yadava**, Vivek Kumar Yadav and Ramesh Kumar Yadav. *RSC Adv.*, **7** (2017) 15917-15925. (IF: 3.2)
35. Anti-leishmanial and cytotoxic activities of amino acid-triazole hybrids: Synthesis, biological evaluation, molecular docking and in silico physico-chemical properties, Mir Mohammad Masood, Phool Hasan, Shams Tabrez, Md Bilal Ahmad, **Umesh Yadava**, Constantin G Daniliuc, Yogesh A Sonawane, Amir Azam, Abdur Rub, Mohammad Abid, *Bioorg. Med. Chem. Lett.*, **27**(9) (2017) 1886-1891. (IF: 2.8)
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72. Investigation of ritonavir analogs antiretroviral natural compounds against SARS-CoV-2 envelope protein, Shivani Negi, Nitin Kumar Kamboj, Gireesh Babu K. & **Umesh Yadava**, Journal of Biomolecular Structure and Dynamics, 2023, DOI:10.1080/07391102.2023.2283872
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(III) Publications in Proceedings

74. Conformational and intramolecular π - π interaction studies on a pyrazolo[3,4-d]pyrimidine derivative, **Umesh Yadava**, Maheshwer Singh, Mihir Roychoudhury, *Proceedings of Emerging Interfaces of Physics and Technology*, Excel India Publishers, New Delhi (2011), 284-289. (ISBN: 978-93-81361-31-3)
75. MD simulation of DNA duplex, Analog of PPT, Its conformation and Hydration: A theoretical Study. Ramesh K. Yadav and **Umesh Yadava**, *Proceedings of Emerging Interfaces of Physics and Technology*, Excel India Publishers, New Delhi (2011), 290-296. (ISBN: 978-93-81361-31-3)

76. Docking Studies of Two Taxane Diterpenoids (10,13-Deacetyl-Abeo-Baccatin-Iv And 5-Acetyl- 2-Deacetoxydecinnamoyl-Taxinine-0.29hydrate) with Microtubule, **Umesh Yadava***, Hariom Gupta and M. Roychoudhury, *Journal of Natural Science, Biology and Medicine* 2(2) (2011) 62. ISSN: **2229-7707**
77. Pyrazolo[3,4-d]pyrimidines as major groove binders: Insight from docking and MD simulations. **Umesh Yadava**, Hariom Gupta, Ramesh K. Yadav and M. Roychoudhury. *Proceedings of National Conference on Nanomaterial and Renewable Energy sources*, JMI, New Delhi (2014) A220, 504-506 (ISBN: 978-93-81212-65-3)
78. Study of 2D Quantitative Structure Activity Relationship of some pyrazolo[3,4-d]pyrimidine derivatives, **Umesh Yadava** and Bindesh Kumar Shukla, *Proceedings of nanotechnology and material science* (2014), 383-386. (ISBN: 978-93-84224-01-1)
79. Quantum Polarized Ligand docking simulation on some Novel inhibitor of Mycobacterium Tuberculosis, Bindesh Kumar Shukla and **Umesh Yadava**, *Proceed. of National conference On Recent Advances in Chemical and Material Sciences*, (2015) 23-24.(ISBN: 978-93-84224-25-7)
80. Characterizations of solute binding proteins by DSF scanning and crystallography, **Umesh Yadava**, Matthew W. Vetting, Steven C. Almo, *Acta Cryst.* (2017), A70, C156 (**IF: 5.725**).

(IV)- Symposium/Conference Presentations

1. **U. Yadava**, M. Roychoudhury and P. R. Maulik, *38th National Seminar on Crystallography* organized by DOS in Geology, University of Mysore, Mysore, INDIA (February 11-13, 2009). Crystallographic evidence for the tolerance of strong electron donating groups on the robustness of the U-motif in pyrazolo[3,4-d]pyrimidine core based dissymmetrical 'Leonard/propylene' linker compounds
2. M. Roychoudhury, **U. Yadava**, and D.K. Gupta *4th National Symposium on Liquid Crystals* organized by Department of Physics, Lucknow University, Lucknow, INDIA (October, 2009). Theoretical investigations on molecular structure and IR frequencies of 4-alkyl-4'-cyano-biphenyl (C₉H₁₉-C₆H₄-C₆H₄-CN) in light of experimental results
3. **U. Yadava**, M. Roychoudhury, C. Ramakrishnan and D. Velmurugan, *4th International symposium on Recent trends in Macromolecular Structure and Function* organized by Centre for Advance Studies in Crystallography and Biophysics, Madras University, Chennai (Jan 21-23, 2010). A comparative study of Crystallographic versus DFT optimized geometry on two taxane diterpenoids and Docking study with Phospholipase A2
4. **U. Yadava**, M. Roychoudhury and M. Singh *Symposium on recent Trends in Biophysics and Workshop on Emerging Techniques of Biophysics* organized by Department of Physics, BHU, Varanasi (Feb. 13-15, 2010). Conformational Studies on 1,3-bis(4-ethoxy-6-methylsulfanyl-1H-pyrazolo[3,4-d]pyrimin-1-yl)propane
5. **U. Yadava**, Poster presentation in the *Workshop on Molecular Modelling and Drug Design* organized by Center for Modelling Simulation and Design, University of Hyderabad (Aug. 2-7, 2010)
6. **U. Yadava**, H.O. Gupta and M. Roychoudhury, *7th Asian Biophysics Association Symposium and Annual Meeting of the Indian Biophysical Society* organized by Department of NMR and MRI Facility, AIIMS, New Delhi, INDIA (Jan28.-Feb.1, 2011). A comparison of Crystallographic versus DFT optimized geometry on two taxane diterpenoids and Docking study with Phospholipase A2.
7. **Umesh Yadava**, Hariom Gupta & Mihir Roychoudhury, *Emerging Interfaces of Physics and Technology*, held at School of Studies in Physics, Vikram University, Ujjain (March 28-30, 2011), A comparative study of crystallographic Vs DFT optimized geometries on two taxane diterpenoids and docking studies with phospholipase A2,
8. **Umesh Yadava**, *Annual Meeting of The Indian Biophysical Society-2012* organized by CAS in Crystallography and Biophysics, University of Madras, Guindy campus, Chennai (January 19-21, 2012). Study of conformational stabilities and intramolecular pi-pi interaction energies of some pyrazolo[3,4-d]pyrimidines.
9. **Umesh Yadava**, *5th International Symposium on Recent Trends in Macromolecular Structure and Function* organized by CAS in Crystallography and Biophysics, University of Madras, Guindy campus, Chennai (January 23-25, 2012). Molecular Docking of Taxane Diterpenoids with Microtubule.
10. **Umesh Yadava**, *National Symposium on Frontiers of Biophysics, Biotechnology, Bioinformatics and 37th Annual Meeting of Indian Biophysical Society* organised by Department of biophysics and center for

excellence in Basic Sciences, University of Mumbai(Jan 13-16, 2013) Pyrazolo[3,4-d]pyrimidines as the inhibitor of anticoagulation and inflammation activities of Phospholipase A2

11. **Umesh Yadava**, *The third Indo-German Conference on Modeling Chemical and Biological (Re)activity* jointly organized by NIPER Mohali and IISER Mohali (Punjab), India (Feb. 26 to March 1, 2013). Pyrazolo[3,4-d]pyrimidines as major groove binders.
12. **Umesh Yadava**, Bindesh K Shukla, M. Roychoudhury, Recent advances in Computational drug design during September 16-17, 2013 organized by Indian Institute of Science, Bangalore and Schrodinger. Pyrazolo[3,4-d]pyrimidines as antiamebic agents: insight from docking and MD simulations.
13. **Umesh Yadava** and Bindesh Kumar Shukla, National conference on Material Science and Technology, March 3-4, 2014 at MMEC Gorakhpur. Study of 2D Quantitative Structure Activity Relationship of some pyrazolo[3,4-d]pyrimidine derivatives
14. **Umesh Yadava**, Hariom Gupta and Ramesh Kumar Yadav. Pyrazolo[3,4-d]pyrimidines as the major groove binders: a computational study. National Conference of Nanotechnology and Renewable energy during March 5- 6, 2014 organized by Jamiya Millia Islamiya Central University, New delhi
15. **Umesh Yadava**, Mihir Roychoudhury. Docking, ADME/T and Molecular Dynamics simulation on some taxane diterpenoids as microtubule stabilizers.59th annual meeting of American Biophysical Association. Feb. 7-11, 2015 at Baltimore, Maryland, USA.
16. **Umesh Yadava**, Matthew W. Vetting, Nawar Al-Obaidi, Steven C. Almo, Structural and Functional Characterizations of Solute binding Proteins by Differential Scanning Fluorimetry and Crystallography. American Crystallographic Association Meeting 2015, Philadelphia, PA, USA from July 25 to 29, 2015
17. **Umesh Yadava** and Sanjai Kumar Yadav, Theoretical Investigations on the molecular structure and IR frequencies of 2,5-bis[4-(N-cyclohexyl-amidino)phenyl]furan. at International conference on Advance in light technologies and spectroscopy of Materials, organized by Department of Physics, Lucknow University,Lucknow held during Jan 16-18, 2016
18. **Umesh Yadava**, Structural and functional characterization of an amino-sugar binding ABC transporter solute binding protein. National conference on Functional Materials held at Department of Physics, DDU Gorakhpur university during March 10-12, 2016
19. **Umesh Yadava**, Mihir Roychoudhury, Novel antitubulin agents from botanical extracts: insight from molecular modeling study, Indian Science Congress Association meeting (Physical sciences section) held at Sri Venkateswera University, Tirupati during January 3-7, 2017.
20. **Umesh Yadava**, Matthew W. Vetting, Characterizations of Solute Binding Proteins by DSF scanning and Crystallography, International union of crystallography, held at International convention center, Hyderabad during August 21 to 28, 2017.
21. **Umesh Yadava**, Computational studies, IR assignments and Molecular docking of 2,5-bis{[4-(n-cyclopropyldiaminomethyl)phenyl]}furan binding with DNA duplex. National Symposium on Multidimensional Aspects of Spectroscopy, organized by Department of Physics, DDU Gorakhpur University, Gorakhpur during November 17-18, 2017.
22. Solute Binding Proteins as Smart Biomolecules: Structural and Functional Characterizations

(VI)-Workshop/Short term course attended

1. **Workshop** on “**Molecular Modeling and Drug Design**” at Centre for Modelling Simulation and Design, University of Hyderabad held from August 2nd to 7th, 2010.
2. **SERC School** lecture on “**Biophysics in Medicine: Advanced Training in Imaging of Experimental Models**” held on 3rd Feb, 2011 organized by Department of NMR and MRI Facility, AIIMS, New Delhi, INDIA
3. Participated in the workshop on “**Proteins to Proteomes: Bioinformatics approach**” organized by Bioinformatics center, University of Pune (Dec. 16-19, 2011).
4. Short term course on “**Water**”, in the Department of zoology, DDU Gorakhpur University Gorakhpur from Dec 17-23, 2013
5. **Orientation course for program officers of NSS**, organized by Gorakhpur empanelled training institute under Department of Youth Affairs, Ministry of youth affairs and sports, Govt. of India from 22.09.2013 to 28.09.2013.