

## Dr. M. VASAVI

M. Sc., Ph. D.

Associate Professor  
University College of Science, Saifabad,  
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### Objective:

To take up a challenging position in the field of computational drug discovery and add value to the existing knowledge of protein-specific targeted therapy for current diseases.

### EDUCATION

- ◆ **Ph.D.**, in **Chemistry**, Osmania University, Hyderabad, INDIA (Feb 2012).
- ◆ **M.Sc., Physical Chemistry**, Osmania University, Hyderabad, INDIA (June 2005)
- ◆ **B.Sc., Food and Nutrition, Food Science and Quality Control, Chemistry**, Osmania University College for Women, Hyderabad, INDIA (April 2003).
- ◆ **Intermediate** St. Pious X Junior College, Hyderabad, INDIA (1998).
- ◆ **10<sup>th</sup> Standard**, The Secondary School Certificate (SSC) (1996).

### PROFESSIONAL EXPERIENCE

#### Teaching Experience – 21 Years

- ◆ Currently working as an **Associate Professor** at University College of Science, Saifabad Osmania University, Hyderabad – 500004 (**From Sep 2025 to Till date**).
- ◆ **Assistant Professor** at University College of Science, Saifabad Osmania University, Hyderabad – 500004 (**From Dec 2013 to Sep 2025**).
- ◆ Worked as **Assistant Professor** at Nizam College, Osmania University, Basheerbagh, Hyderabad - 500001 (From Sep 2013 to Dec 2013).
- ◆ **Assistant Professor (C)**, at the Department of Chemistry, Nizam College, Osmania University, taught B. Sc. and M. Sc. courses in Chemistry (2007- 2009).
- ◆ **Assistant Professor (Part-time)** at Department of Chemistry, Nizam College, Osmania University, Hyderabad, and University College for Women, O.U., Hyderabad, taught M.Sc. and B.Sc. courses in Chemistry. (2005 - 2007)

#### Research Experience - 20 years

- ◆ **Supervising Ph.D. students**  
Recognised research guide for Ph.D. Students in Chemistry and other allied areas of research at Osmania University.

#### Ph.D. Thesis submitted/Awarded

1. Ms. B. Madhavi Latha, Computationally aided discovery of Novel lead molecules, Submitted thesis in April 2025.
2. Ms. G. Priyadarshini, Fold-Based 3D model generation of proteins: Insilico identification of strong inhibitors against Cancer, Submitted thesis in September 2025

#### Ph.D.'s Awarded.

1. Dr. D. Thirupathi, Design novel lead molecules using molecular modeling techniques, Osmania University, 13 Feb 2026.
2. Dr. K. Vani, Application of In silico drug designing techniques to identify Novel lead molecules, Osmania University, 21 Feb 2026.
3. Application of Computational Techniques for Designing Novel Lead Molecules against Tuberculosis, Dr. B. Mounika, Osmania University, 10 Jan 2025.
4. Identification of novel lead molecules for tuberculosis targets by applying computer-aided drug discovery techniques, Dr. R. Lavanya, Osmania University, 25 Sep 2024.
5. Thesis entitled Application of Computational Techniques for Identification of Novel Molecular Entities, Ramesh Malikanti, Osmania University, Oct, 2022.

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### M.Sc. Dissertation

1. Pharmacological evaluation and pharmacophore model of oxadiazoles as anti-alzheimer's agents (S. Prasad, K. Supriya, S. Nandini, M. Sindhuja, and Nikhath Fathima, Project Dissertation submitted to UCSS, Osmania University, Dec 2025)
2. ADME and toxicity prediction of octaprenyl transferase inhibitors of *Mycobacterium tuberculosis*, (P. Kalyani, and Amthul Muneer Ayesha, Project Dissertation submitted to, Osmania University, Nov 2025)
3. Computational studies of KS1 protein biomarker for lung adenocarcinoma, M. Kavya Sri and Ramya G (Project Dissertation submitted to, Loyola Academy, Old Alwal, Dec, 2022)

1<sup>st</sup> Aug 2011-Sep 2013 worked as a **Scientist, Computational Chemistry** in Synthetic division, **United States Pharmacopoeia India Pvt. Ltd**, Shameerpet, Hyderabad, India.

### Job responsibilities include

- Quantum Chemical calculations: (DFT) Determination of the feasibility of reactions.
  - Quantum Chemical calculations application in the organic synthesis R&D
  - Literature search and root selection of the organic reactions for synthesis
  - Establishment of computational facility
- ◆ **Ph.D.** in Chemistry "Design of new chemical entities for novel therapeutic targets of *Mycobacterium tuberculosis* - A computational approach" (Feb 2012), Osmania University.
  - ◆ Worked as a Research fellow in the UGC-sponsored research project entitled "A Novel therapeutic target for tuberculosis – Identification of new lead molecule", F.No. 34 302/2008 (SR); Mar 2009-Jul 2011.
  - ◆ Patents : Published- **3**
  - ◆ Research Grants : **1** (UGC BSR start-up grant)
  - ◆ Number of Ph.Ds Awarded: **5** ; Thesis submitted : **2**
  - ◆ Number of students registered for Ph.D.: **0+2** students: **7** Students (M.Sc. Project)
  - ◆ Project Mentor : **5** Projects (Annexure III)
  - ◆ Publications : International Published-**35** (Annexure I)
  - ◆ Conference proceedings : **5** (Annexure I)
  - ◆ Workshops attended : **16-** workshops (Annexure II)
  - ◆ Guest Speaker : **4** (Annexure II)
  - ◆ Conference Presentations : International-**28**, National-**10** (Annexure II)
  - ◆ Organising committee member of conferences: **4**-conferences
  - ◆ Collaborations : **3** (Annexure III)

**Project** UGC Start-Up grant of Rs. 600000/-UGC order No. F. 30 – 108/2015 (BSR), entitled Computational design of Novel leads as inhibitors of *Mycobacterium tuberculosis* proteins

### Member of Academic Bodies

- ◆ Indian Science Congress Association (L33317)
- ◆ Associate Fellow (2020), Telangana Academy of Science

### Administrative and Academic positions held

- ◆ I/c Head, Department of Chemistry, University College of Science, Saifabad, OU.
- ◆ Hostel Mess Warden, Ladies Hostel, CHW-IV, OU.
- ◆ Academic Coordinator, University College of Science, Saifabad, Hyderabad-500004.
- ◆ I/c NCC officer, University College of Science, Saifabad, OU, Hyderabad – 500004.

### AWARDS

- ◆ Best Researcher Award, 2023, University College of Science, Saifabad, OSMANIA UNIVERSITY, Hyderabad.

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- ◆ 2020, Associate fellow, Telangana Academy of Science, Telangana, INDIA.
- ◆ Science Seva Ratna Award". Gandhi Global Family, Gandhi Gnana Pratishtan on the occasion of National Science Day - 2021 held on 28<sup>th</sup> Feb' 2021 at B.M. Birla Science center, Hyderabad, Telangana State, INDIA.
- ◆ Best poster prize for "Identification of Novel Serpins as Inhibitors of SP1 Protein – An *In silico* Approach" at NIT Warangal International conference on advances in chemical sciences and technologies during 23<sup>rd</sup> to 25<sup>th</sup> Sep 2019
- ◆ Young Scientist Award - 2010 in Chemistry & Allied Sciences by Dr. K.V. Rao Scientific Society, Hyderabad, India.
- ◆ Best poster prize for "Potent target for cancer therapy" in 4<sup>th</sup> Indo US Lecture series on Discrete Mathematical Chemistry (6-9<sup>th</sup> January 2009).

### SOFTWARE SKILLS

#### ◆ Computer Skills

Operating systems Windows 10, 8, 7 / Vista /XP/2000,  
Linux RedHat/Suse/Fedora/ Centos

#### ◆ Molecular Modeling Software Packages

Quantum mechanics	Gaussian09 and GaussView05
Statistical	SPSS
Homology modeling	Modeller, ProSA, Procheck.
Active site	Site Map (Schrodinger suite), Q – Site, CASTp
Docking	Glide, Autodock, Vina, PyRx, FlexX, HEX, VEGAZZ, Argus lab, Gold, Chemaxon, ZDOCK
Molecular Dynamics	NAMD, VMD, Desmond
Pharmacophore Mapping	Phase (Schrodinger suite)
Visualization & Sketching	Meastro, Rasmol, Spdbv, Pymol, Mercury, Chimera,
Tools	Discovery Studio Visualiser, VMD, ChemSW, Chemdraw, ISISdraw, ACD labs, ChemBioOffice
ADME predictions	QikProp (Schrodinger suite)

#### ◆ Databases

Nucleotide databases	Genebank NCBI, DDBJ Nucleotide sequence database (EMBL)
Protein Data Bases	NCBI, ExPasy-UniProt Knowledgebase
Metabolic database	KEGG, RoChie, Biocarta
Structural database	PDB, CATH, SCOP, PDBe
Small molecules	ZINC, NCDB, ChEMBL, Cambridge Structural Database

### EXTRA CURRICULAR ACTIVITIES

- ◆ Awarded National Cadet Corps (NCC) 'C' Certificate.
- ◆ Represented College at the Inter College Volleyball competition.

### PERSONAL DATA

- ◆ DOB 22<sup>nd</sup> March 1981, INDIAN.
- ◆ Married and Two Children
- ◆ Ever willing to learn, Positive Attitude, Planning and Executing skills, Creative, Team spirit, Research bent of Mind, Goal Oriented, Healthy, Strong, Sincere, and Self-Motivated.

**REFERENCES:** Available upon request

(Dr. M. VASAVI)

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**ANNEXURE - I**

**LIST OF PATENTS/ PUBLICATIONS**

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**Patents:**

- 1. NOVEL SCHIFF BASE DERIVATIVES.** Uma Vuruputuri, Vasavi Malkhed, Kiran Kumar Mustyala, Sarita Rajender Potlapally, Ramasree Dulapalli, Srinand Sreevatsan, Anthony David Baughn. **Indian Patent application number – 6190/ CHE/ 2014 Patent no: IN 315635** (Publication Date: 26/08/2016).
- 2. Design, Synthesis and Cytotoxic Studies of Piperazine Derivatives against Cancer.** Uma Vuruputuri, Sarita Rajender Potlapally, Vasavi Malkhed, Kiran Kumar Mustyala, Ramasree Dulapalli, V.G.M. Naidu. **Indian Patent application number 5681/CHE/ 2014** (Publication Date: 19/12/2014)
- 3. Synthesis and Cytotoxic Studies of Barbituric Acid Derivatives.** Uma Vuruputuri, Sarita Rajender Potlapally, Bhargavi Kondagari and Vasavi Malkhed, **Indian Patent application number 3345/CHE/2012** (Publication Date: 07/03/2014)

**Publications:**

**Citations – 319**

**H- Index – 11**

**I10-index – 14**

1. An In Silico Design, Simulation, Virtual Screening, and Evaluation of Natural Products as Inhibitors of Breast Cancer-Causing Kallikrein11 Protein and Comparison of Binding Affinities with Approved Drugs. (Accepted for publication in Current Drug Targets) (IF: 2.5) ISSN (Print): 1389-4501/ISSN (Online): 1873-5592 (Q2 Journal)
2. Sagar Rout, Katarina Bauerova, Bhabani Sankar Satapathy, Srikanth Gatadi, **Vasavi Malkhed**, (2025), Unveiling Anti-Cancer Potential through ADMET Prediction, Molecular Docking, Molecular Dynamics, and In vitro Analysis: Approach to Establish Alpha-Terpineol as a Potential Drug Candidate against Glioma." Current topics in medicinal chemistry, (<https://doi.org/10.2174/0115680266386465250702204827>) (IF: 3.3) (Q2 Journal).
3. A. Mishra, B. Sankar Satapathy, S. Gatadi, **M. Vasavi**, P. Kumar Sahu, V. Nuthakki, (2025) Garcinol as A Promising Therapeutic Candidate for Alzheimer's Disease: Integrated Computational and In Vitro Target Analysis. ChemistrySelect, (10) e01371. (<https://doi.org/10.1002/slct.202501371>) (IF: 2) (Q3 Journal).
4. Sravanthi Maddikayala, Kavitha Bengi, **Vasavi Malkhed**, Saritha Reddy Pulimamidi\* (2025), In Silico Docking Studies, ADMET Properties, DNA Interaction, and Biological and in Vivo Anti-Inflammatory Studies of Schiff Base Metal Complexes Derived From o-Hydroxyacetophenone. Appl. Organomet. Chem., 39: e7949. (<https://doi.org/10.1002/aoc.7949>) (IF: 0) (Citations: 3). (Q2 Journal)
5. Lavanya Rumandla, Mounika Badineni, Ramesh Malikanti, Rajender Vadija, Kiran Kumar Mustyala & **Vasavi Malkhed**, (Jun 2024), Virtual Screening Technique to Identify

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- Inhibitors of Mycobacterium tuberculosis Rv3032 Protein Involved in MGLP Biosynthesis, Russian Journal of Bioorganic Chemistry, 50, (3) 1067-1081. (DOI: 10.1134/S1068162024030300) (IF: 1.7) (Citations: 3). (Q4 Journal)
6. Hareesh Reddy Badepally, Lavanya Rumandla, Mounika Badineni, Ramesh Malikanti, Rajender Vadija, Kiran Kumar Mustyala, **Vasavi Malkhed\***, (2024) Design of molecular inhibitors against the NuoC protein of Mycobacterium tuberculosis (May 2024), International Journal of Pharmaceutical Sciences and Drug Research, 16, (3) 308-322. (DOI: 10.25004/IJPSDR.2024.160302) (IF: 0) (Citations: 0). (Q4 Journal)
  7. Chintalapati, Krishnam Raju, Yesudas Kada, **Vasavi Malkhed**, Sanath Kumar Goud Palusa, Rabin Bera, and V. Shanmukha Kumar Jagarlapudi, (**Mar 2024**) In silico Studies of Cilnidipine Degradation Products for Structure Confirmation, Toxicity Prediction and Molecular Docking Authors, Asian Journal of Chemistry, 36, (4) 865-878. (DOI: 10.14233/AJCHEM.2024.31150) (IF: 0.156) (Citations:). (Q4 Journal)
  8. Badineni, Mounika; **Malkhed, Vasavi\***; Rumandla, Lavanya; Malikanti, Ramesh; Vadija, Rajender; Mustyala, Kiran K, (**Sep 2023**), Structure Elucidation and Identification of Novel Lead Molecules against Sulfur Import Protein cysA of Mycobacterium tuberculosis, Current Protein & Peptide Science, 24, (7) 589-609 (DOI: 10.2174/1389203724666230713124339) (IF: 2.5) (Citations: 3). (Q4 Journal)
  9. Chivukula, Sowmya; **Malkhed, Vasavi\***, (**Aug 2023**), The Role of CDK20 Protein in Carcinogenesis, Current Drug Targets, 24, (10) 790-796 (DOI: 10.2174/1389450124666230719102112) (IF: 2.5) (Citations: 10). (Q2 Journal)
  10. Damera, Thirupathi; Kondaparthi, Vani; Bingi, Madhavi Latha; Mustyala, Kiran Kumar; **Malkhed, Vasavi\***; (2023) Identification of novel scaffolds to inhibit Mycobacterium tuberculosis PimA protein—A computational approach, Journal of Cellular Biochemistry, 124 (6) 836-848 (DOI: 10.1002/jcb.30412) (IF: 2.8) (Citations: 7). (Q2 Journal)
  11. Jyothi Bandi, **Vasavi Malkhed** & Navaneetha Nambigari, (**2022**), An insilico study of KLK-14 protein and its inhibition with curcumin and its derivatives, Chemical Papers, 76, 4955–4966 (<https://doi.org/10.1007/s11696-022-02209-w>), (IF: 2.14) (Citations: 2). (Q2 Journal)
  12. Structural determination of plasma kallikrein protein and identification of its inhibitors in cancer: an in-silico study, (Jan 2022), Vani Kondaparthi, Madhavi Latha Bingi, Thirupathi Damera, Priyadarshini Gangidi, Mounika Badineni, Kiran Kumar Mustyala, & **Vasavi Malkhed\***. Journal of Population Therapeutics and Clinical Pharmacology, 29(01), 625-648. (<https://doi.org/10.53555/94hryg02>) (IF:) (Citations:0).
  13. Madhavi Latha Bingi, Vani Kondaparthi, Thirupathi Damera, Priyadarshini Gangidi, Hareesh Reddy Badepally, Mounika Badineni, Kiran Kumar Mustyala, & **Vasavi Malkhed\***, (2021), Exploring innovative inhibitor candidates targeting the rhoG protein: an in-silico investigation, 2021, Journal of Population Therapeutics and Clinical Pharmacology, 28(2), 706-724. (<https://doi.org/10.53555/pab6y090>) (IF:) (Citations:0).

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14. Narendra Kumar Maddali, V. Kasi Viswanath Ivaturi, L. N. Murthy Yellajosula, **Vasavi Malkhed**, Pradeep Kumar Brahman, Sai Kiran S. S. Pindiprolu, Vani Kondaparthi, Sundara Rao Nethinti, (2021), New 1,2,4-Triazole Scaffolds as Anticancer Agents: Synthesis, Biological Evaluation, and Docking Studies, **ChemistrySelect**, **6, 26, 6788-6796** (<https://doi.org/10.1002/slct.202101387>)(**IF: 2.109**) (Citations:18). (Q2 Journal)
15. Maddali, N. K., Viswanath, I. V. K., Murthy, Y. L. N., **Malkhed, V.**, Kondaparthi, V., Brahman, P. K. and Govindh, B., (2021), Novel Pyrimidinone Linked 1,2,3-Triazole Scaffolds as Anti-Microbial and Antioxidant Agents: Synthesis, In-vitro and In-silico Studies, **Journal of Pharmaceutical Research International**, **33,59A, 477-491.** (doi: 10.9734/jpri/2021/v33i59A34295) (**IF: 0**) (Citations: 2).
16. Tejeswara Rao Allaka, Naresh Kumar Katari, Sreekantha B. Jonnalagadda, **Vasavi Malkhed**, Jaya Shree Anireddy, (2021), Design, Synthesis and Biological Evaluation of Novel Heterocyclic Fluoroquinolone Citrate Conjugates as Potential Inhibitors of Topoisomerase IV: A Computational Molecular Modeling Studies, **Current Drug Discovery Technologies**, **18, 6, 78 - 97.** (<https://doi.org/10.2174/1570163817666201106143557>) (**IF: 1.2**) (**Citations: 2**). (**Q3 Journal**)
17. Hymavathi Veeravarapu, Vasavi Malkhed, Kiran Kumar Mustyala, Rajender Vadija, Ramesh Malikanti, Uma Vuruputuri, Murali Krishna Kumar Muthyala, (2021), Structure-based drug design, synthesis and screening of MmaA1 inhibitors as novel anti TB agents, *Molecular Diversity*, **25, 1, 351-366.**(<https://doi.org/10.1007/s11030-020-10107-0>) (**IF: 2.032**) (Citations: 21). (Q2 Journal)
18. Vadija R, Mustyala KK, **Malkhed V**, Dulapalli R, Veeravarapu H, Malikanti R, Vuruputuri U, (2018), Identification of small molecular inhibitors for efflux protein Rv2688c of Mycobacterium tuberculosis, **Biotechnol Appl Biochem**, **608-621.** (**IF: 1.413**) (Citations: 4). (Q2 Journal)
19. Rajender Vadija, Hymavathi Veeravarapu, Kiran Kumar Mustyala, **Vasavi Malkhed**, Uma Vuruputuri, (2017), Identification of small molecular ligands as potent inhibitors of fatty acid metabolism in Mycobacterium tuberculosis, Ramesh Malikanti, **Journal of Molecular Structure** **1150, 227 - 241.** (**IF: 1.75**) (Citations: 10). (Q2 Journal)
20. MK Metta, **V Malkhed**, S Tantravahi, U Vuruputuri, R Kunaparaju, (2017), Development of an in vitro Bioassay for Recombinant Human Erythropoietin (rHuEPO) Based on Proliferative Stimulation of an Erythroid Cell Line and Analysis of Sialic Acid Dependent Microheterogeneity: UT-7 Cell Bioassay, MK Metta, **V Malkhed**, S Tantravahi, U Vuruputuri, R Kunaparaju,2017, **The Protein Journal**, **36, 112-122.** (**IF: 1.139**) (Citations: 25). (Q3 Journal)
21. Thirupathi, D., Bhargavi, K., Ramasree, D., Aboubakr H. A., Thirupathi M., Lavanya, S. P.R., **Vasavi, M.**, Uma V., (2017), Design of novel lead molecules against RhoG protein as cancer target-a computational study, **Journal of Biomolecular Structure and Dynamics**, **35, 14, 3119-3139** (**IF: 3.12**) (Citations: 11). (Q2 Journal)

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22. Identification of Small Molecular Inhibitors for Efflux Protein: DrrA of Mycobacterium tuberculosis, Kiran, K. M., **Vasavi, M.**, Venkataramana, R. Ch., Uma V. **Cel. Mol. Bioeng. 2016, 9 (1), 190-202 (IF: 2.535)** (Citations: 5). (Q2 Journal)
23. Virtual screening studies to identify novel inhibitors for Sigma F protein of Mycobacterium tuberculosis, Kiran, K. M.; **Vasavi, M.**; Venkataramana, R. Ch.; Uma, V. **I. J. Myco. 2015, 4 (4), 330-336 (IF: 0.53)** (Citations: 11). (Q3 Journal)
24. Macromolecular structure and interaction studies of SigF and Usfx in Mycobacterium tuberculosis. Kiran, K. M.; **Vasavi, M.**; Sarita, R. P.; Venkataramana Reddy, C.; Uma, V. **J. Recept. Signal. Transduct. Res. 2014, 34, 3, 162-173. (IF: 1.61)** (Citations:10). (Q3 Journal)
25. Identification of novel leads applying in silico studies for Mycobacterium multidrug-resistant (MMR) protein. **Vasavi, M.**; Kiran, K. M.; Sarita, R. P.; Uma, V. **J. Biomol. Struct. Dyn. 2013, 32, 1889-1906. (IF: 3.12)** (Citations: 19). (Q2 Journal)
26. A Molecular Dynamic Simulations of Co (III) and Ru (II) polypyridyl complexes and its docking studies with dsDNA. Navaneetha, N.; Nagababu, P.; Kiran, K. M.; **Vasavi, M.**; Ramasree, D.; Satyanarayana,S.; Uma, V. **Med. Chem. Res. 2013, 22, 5557-5565. (IF: 1.27)** (Citations: 18). (Q2 Journal)
27. Modeling of alternate RNA polymerase sigma D factor and identification of novel inhibitors by virtual screening, **Vasavi, M.**; Kiran, K. M.; Sarita, R. P.; Uma, V. **Cel. Mol. Bioeng. 2012, 5, 363-374. (IF: 2.535)** (Citations: 9). (Q2 Journal)
28. The 3D-structural evaluation and binding of AIFM2 to DNA: An insilico study. Ramasree, D.; Satyaprakash, A.S.V.; Bhargavi, K.; **Vasavi, M.**; Uma, V. **J. Pharmacy Research. 2012, 5, 3099. (IF: 2.36)**
29. Novel inhibitors targeting cell signaling receptor – cyclin D2 by virtual screening.Sarita, R. P.; Kiran, K. M.; **Vasavi, M.**; Uma, V. **J. Pharmacy Research. 2012, 5, 572. (IF: 2.36)** (Citations: 4).
30. Angiogenesis: an insilico approach to angiogenic phenotype.Navaneetha, N.; Kiran, K. M.; **Vasavi, M.**; Bhargavi, K.; Sarita, R. P.; Ramasree, D.; Uma, V. **J. Pharmacy Research. 2012, 5, 583. (IF: 2.36)** (Citations: 6).
31. Study of interactions between **Mycobacterium tuberculosis proteins - Sig K and anti - Sig K. Vasavi, M.**; Bargavi, G.; Bhargavi, K.; Ramasree, D.; Uma, V. **J. Mol. Model. 2011, 17, 1109. (IF: 1.86)** (Citations: 14). (Q3 Journal)
32. Identification of novel selective antagonists for cyclin C by Homology modeling and virtual screening.Sarita, R. P.; **Vasavi, M.**; Uma, V. **Int. J. Biol. Macromol. 2011, 48,292. (IF: 3.09)** (Citations: 26). (Q3 Journal)
33. Homology Modeling and Docking Studies of Human Bcl-2L10 protein.Bhargavi, K.; Kalyan, C. P.; Ramasree, D.; **Vasavi, M.**; Murthy, D. K.;Uma, V.**J. Biomol. Struct. Dyn. 2010, 28, 379. (IF: 2.98)** (Citations: 36). (Q2 Journal)

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34. Selective Inhibition of Proteins Regulating CDK / Cyclin Complexes: Strategy Against Cancer – A Review. Sarita, R. P.; Ramasree, D.; Bhargavi, K.; **Vasavi, M.**; Uma V.J. **Recept. Signal. Transduct. Res.** **2010, 30, 206. (IF: 1.61)** (Citations:33). (Q3 Journal)
35. Tricyclic Pthalimide Analogues as Novel Inhibitors of HIV-1 Integrase – A QSAR Study. **Vasavi, M.**; Kalyan, C. P.; Ramasree, D.; Sarita, R.; Uma, V. **Bioinformatics Trends.** **2007, 2, 61. (IF: Not available)** (Citations:).
36. Multi drug resistant protein of Mycobacterium tuberculosis 3D Homology model. **Generated and deposited in Protein Data Bank with PDB ID - 2IQ4. Vasavi, M.**; Kalyan, C. P.; Ramakrishna, A.; Uma, V. **(Oct - 2006). (IF: Not available)** (Citations:).

### Proceedings:

1. Identification of Novel Molecular Scaffolds as Inhibitors of SP2 Protein-An Insilico Approach. Vani Kondaparthi, Thirupathi Damera, Madhavalatha Bingi, Lavanya Rumandla, **Vasavi Malkhed, Proceedings of International Conference on Drug Discovery (ICDD), SSRN 3529915, 2020.**
2. Targeted therapy for cancer: An In silico approach, Aruna Airva, Upender Bowroju, **Vasavi Malkhed & Navaneetha Nambigari**, Second National Conference on Recent advances in applied nanomaterials, at Department of Physics, University College of Science, Saifabad, Osmania University, Hyderabad, February 16-17, 2018, **International Journal of research culture society, 2018, 47-52. (Impact factor 3.449)**
3. *Small molecule identification against novel MDRA protein of Mycobacterium tuberculosis.* Kiran, K. M.; **Vasavi, M.**; Venkataramana, R. C.; Uma, V.; **J. Biomol. Struct. Dyn.** **2013, 31, 1, 118. (Impact factor 2.98)**
4. *Design of new leads as novel therapeutics for Tuberculosis - A computational approach.* Uma, V.; **Vasavi, M.** 3<sup>rd</sup> World Congress on Biotechnology 2012, organized by Omics group, at HICC, Hyderabad, India on 13-15 September, **2012. J. Biotechnol Biomater** **2012, 2, 6, 155. (Impact Factor: Not available)**
5. *Design and synthesis of potent Cyclin C inhibitors.* Sarita, R. P.; Kiran, K. M.; Bhargavi K.; **Vasavi, M.**; Uma, V. **J. of Bioavailability and Bioequivalence.** **2012, 4, 43. (Impact Factor 2.00)**

### ANNEXURE- II

#### WORKSHOPS ATTENDED

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1. FDP **AI Mastery for Educators**, organised by Vishlesan i-HUB IIT Patna, from 15-05-2025 to 07-06-2025.
2. Three-week certificate course on **Computer-Aided Drug Design (CADD)**, organised by Vidyothini Edutech Pvt Ltd, from 05-05-2025 to 23-05-2025.
3. Three-Day National Workshop on "**NAAC Accreditation and Outcome-Based Education through AI-Powered Digital Learning**", organised by The Office of Dean, Development

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& UGC Affairs, and Internal Quality Assurance Cell (IQAC), Osmania University, Hyderabad-500007, from 03-03-2025 to 5-03-2025.

4. Faculty Training Program '**Workshop on Molecular Docking, Virtual Screening and Computational Biology**, organised by NIPER- Hyderabad, Balanagar, Hyderabad-500037, Telangana, from 26-02-2024 to 08-03-2024 (Skill Vigyan Initiative Scheme of The Department of Biotechnology, Govt. of India, Coordinated by TSCOST).
5. **Drug Discovery and Novel Drug Development -Analytical Interpretation of Research Data**, organised by UGC-MMTTC JNTU-H, from 13-02-2023 to 27-02-2023.
6. **MOOCs, E-Content Development** and Online Pedagogy, organised by UGC-MMTTC JNTU-H, from 31-10-2022 to 05-11-2022.
7. Online Faculty Development program on **Applications of DFT (Density Functional Theory) in Teaching and Learning Chemistry, Physics, and Material Science with software for chemistry and Materials (SCM-AMS)** Organised by the Department of Chemistry, NIT, Warangal and Teaching Learning Centre, of PMMMNMTT, MHRD, Govt. of India, during 19<sup>th</sup> -24<sup>th</sup> March 2021.
8. Online Faculty Development program on **Effective Teaching and Learning of Modern Drug Discovery Approaches**, Organised by the Department of Chemistry, NIT, Warangal and Teaching Learning Centre, of PMMMNMTT, MHRD, Govt. of India, during 4<sup>th</sup> -9<sup>th</sup> March 2021.
9. **Science leadership workshop** organised by the Central University of Panjab, Bathinda, India, from June 22<sup>nd</sup> to 28<sup>th</sup>, 2020
10. SWAYAM ARPIT- **Online Annual refresher course in Chemistry** for higher education faculty conducted by Sri Guru Tegh Bahadur Khalsa College, University of Delhi. (Examination Held on 16-02-2020)
11. Attended 2<sup>nd</sup> **ACS – CRSI meeting 2019** at IIT, Kanpur, INDIA, held on 18<sup>th</sup> Jul 2019.
12. SWAYAM ARPIT- **Online Annual refresher course in Chemistry** for higher education faculty conducted by Sri Guru Tegh Bahadur Khalsa College, University of Delhi 2019.
13. Three-day workshop on teaching pedagogy for **PG Teachers in Chemistry**, 18<sup>th</sup> -20<sup>th</sup> March 2019, Department of Chemistry, University College of Science, Osmania University, Hyderabad
14. Attended International Symposium on **Recent Trends in Chemical Biology** organised by RDCC, O.U., Hyderabad on 28<sup>th</sup> Nov, 2018.
15. **Refresher Course in Chemistry** at UGC-HRDC, University of Hyderabad, Hyderabad, held from 5<sup>th</sup> Sep 2018 to 25<sup>th</sup> Sep 2018.
16. **Refresher Course on "Basic Principles and Research Advancements in Life Sciences and Pharmaceutical Sciences"** at UGC-HRDC, JNTU, Hyderabad, held from 22<sup>nd</sup> Jan 2018 to 12<sup>th</sup> Feb 2018.

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17. **NCC Training course** from 06<sup>th</sup> Sep 2017 to 18<sup>th</sup> Sep 2017 conducted by 1(T) Arty Btl unit, Hyderabad.
18. Workshop on **Protein Structure and Drug Discovery**, organised by the School of Life Sciences, University of Hyderabad, Hyderabad, held from 27<sup>th</sup> Aug 2017 to 05<sup>th</sup> Sep 2017
19. Workshop on **International Conference on Drug Design: ICDD 2017, organised by Schrodinger llc** at JNU Delhi on 7<sup>th</sup>-April 2017.
20. **45<sup>th</sup> Orientation Course** organized by UGC-HRDC, JNTUH, Hyderabad, held from 11<sup>th</sup> Jun 2016 to 08<sup>th</sup> Aug 2016.
21. Work shop on **Introduction to Gaussian: Theory and Practice**, held at Hotel Connaught New Delhi, 37 Shaheed Bhagat Sing Marg, New Delhi, India, Organised by Gaussian, Inc., SCUBE Scientific Software Solutions, the Green Chemistry Network Center, the University of Delhi, and the Royal Society of Chemistry London (North India Section) (17<sup>th</sup>to 21<sup>st</sup> Dec, 2012).
22. Workshop on **Molecular Design** organised by the Department of Chemistry, P.G. College of Science, Saifabad, Osmania University, Hyderabad, India and Schrodinger, India (26<sup>th</sup> and 27<sup>th</sup> April, 2010).
23. Workshop on **user awareness program on access to e-Resources** under the UGC-INFONET digital library consortium, organised by the University Library, Osmania University, Hyderabad, India (23<sup>rd</sup> June 2009).
24. Workshop on **Basic concepts of statistical methods in biological data analysis, Implementation of statistical methods in analysis of genomics, proteomics data and hands on practice using statistical and mathematical packages** at Bioinformatics Statistical School (Bioinformatics Infrastructure Facility), University of Hyderabad, jointly organized by School of Life Sciences and CR Rao Advanced Institute of Mathematics, Statistics and Computer Sciences, University of Hyderabad (UOH), Hyderabad, India (1<sup>st</sup> – 16<sup>th</sup> Dec, 2008)
25. Workshop on **Applications of Artificial Intelligence and Machine Learning in Bioinformatics and Chemo-Informatics** held at The Department of Bioinformatics, Bharathidasan University, Thirichirappalli, Tamilnadu, India (5<sup>th</sup> Nov, 2007).

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### GUEST SPEAKER/ Invited Lectures/Resource person

1. Interactive Evaluation for 31st NCSC-2023, National Participants from (APCOST) AP, 13th December 2023 online from 10:00 am to 2:00 pm.
2. Resource person for evaluation of oral presentations at the International Conference on Recent Innovations in Science and Technology-2023, organized by UCSS, OU (30-09-2023).
3. Chemistry judges panel member for the 12th SPARK Innovation Awards event held on 8th April 2023.

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4. Evaluator for Exhibition of Science Models, finals round on 28th February 2023, organized by KVRSS, in collaboration with Satya Sai Institute of Higher Learning (SSSIHL), Puttaparthi, National-level competitions to celebrate National Science Day- 2023.
5. Resource person in **Virtual Workshop on Collating Chemistry Resources for Teachers in Higher Education** organized by National Resource Centre for Education (June 18-19, 2020) at NIEPA, New Delhi.
6. Dr. M. Vasavi delivered a guest lecture on **Solid State** (12th March 2019) at Keshava Memorial Institute of Commerce and Sciences, Narayanguda, Hyderabad.
7. Dr. M. Vasavi **delivered an extension lecture on Solid State Chemistry** (23rd Feb 2019) at RBVRR Women's College, Narayanguda, Hyderabad.
8. Delivered a talk on '**Identification of New lead molecules using computer-aided modeling studies**' at the Seminar series on molecular modeling and drug designing and docking, 28<sup>th</sup> to 29<sup>th</sup> Jan 2013, held at Department of Biotechnology, Sreenidhi Institute of Science and Technology, Ghatkesar, Hyderabad, 501301.

## SEMINAR / CONFERENCE PRESENTATIONS

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### International Conference

1. Identification of small ligand molecules as potent inhibitors of SK protein against Prostate Cancer Metastasis. Priyadarshini Gangidi<sup>1</sup>, Vani Kondaparthi<sup>1</sup>, Madhavalatha Bingi<sup>1</sup>, Mounik Badineni<sup>1</sup>, **Vasavi Malkhed<sup>1,2\*</sup>** at International Conference on Integrative Trends in Pharmaceutical and Health Sciences, Healthcare Next 2025 organised by GITAMS Deemed to be University from 12 to 14 February 2025.
2. Design and discovery of SP3 protein inhibitors: A Computational approach  
Vani Kondaparthi, **Vasavi Malkhed\*** at "International conference on Recent Innovations in Science and Technology-2023" organised by University College of Science, Saifabad, OU on 30th September, 2023.  
Identification of molecular inhibitors for N1 protein of Mycobacterium tuberculosis. Hareesh Reddy; Madhavi Latha Bingi; Lavanya Rumandla, **Vasavi Malkhed\***. Presented at International conference on "Recent Innovations in Science and Technology" (RIST-2023), 30<sup>th</sup> September, 2023. Organized by University College of Science, Saifabad, Hyderabad.
3. Presented a poster entitled "In Silico Approach for Identifying Natural SM4 Protein Inhibitors to inhibit Lung Adenocarcinoma", Sowmya Chivukula, Kiran Kumar Mustyala, **Vasavi Malkhed**, at International Conference on Drug Discovery 2022 hosted by Schrodinger Inc, USA in collaboration with BITS-Pilani, Goa Campus, on 10<sup>th</sup> and 11<sup>th</sup> Nov, 2022.
4. Presented posters at Current trends and Futuristic challenges in chemical sciences, 29<sup>th</sup> and 30<sup>th</sup> Jul 2022, Department of Chemistry, University College of Science, Osmania University, Hyderabad-500007.
  - i) Understanding the gene paradigm association with COVID-19 loci, Parthiban Karthigan, **Vasavi Malkhed**.
  - ii) Identification of Novel Lead Molecules as R1 Protein Inhibitors—a Computational Study, Madhavalatha Bingi, Mounik Badineni, Lavanya Rumandla, **Vasavi Malkhed**.

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- iii) 3D structure prediction and identification of potential plant-based inhibitors for SP4 protein using in silico studies. SowmyaChivukula, **Vasavi Malkhed.**
  - iv) An in silico attempt for recognition of lead compounds against the DT4 protein of *Mycobacterium tuberculosis*, Thirupathi Damera, Vani Kondaparthi, Madhavalatha Bingi, Kiran Kumar Mustyala, **Vasavi Malkhed.**
5. Presented at Two-Day Virtual International Conference on Chemical Advances for Sustainable Development (CASD-2022) organised by University College of Women Koti, Osmania University during 12 -13<sup>th</sup> April 2022.
- i) Identification of New Lead Molecules against SWM Protein for Cancer Therapy. Sowmya Chivukula, Thirupathi Damera, **Vasavi Malkhed.**
  - ii) Unfolding the 3d structure of the ksk2 protein and identifying novel scaffolds against it: a paradigm for discovering new tb therapeutics. Mounika Badineni, Lavanya Rumandla, Vani Kondaparthi, Madhavalatha Bingi, Rajender Vadija, **Vasavi Malkhed.**
6. Presented poster at Virtual Winter workshop on Multiscale modeling on Nov 22-23, 2021, by Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany.
- i) Homology modelling and identification of novel leads against the KSK1 protein: A strategy to explore new Tuberculosis therapeutics. Mounika B, Lavanya R, Ramesh M, Rajender V, Kiran Kumar M, **Vasavi M.**
7. Presented poster at International Conference on CDMCE-2021 by NIT Warangal from 29-31 July 2021
- i) An insilico approach for identification of novel lead compounds against the DT2 protein of *Mycobacterium tuberculosis*, Thirupathi Damera, Vani Kondaparthi Madhavalatha Bingi, Kiran Kumar Mustyala, **Vasavi Malkhed.**
8. Presented a poster at the International Conference on Material Science for Societal Advancement, Osmania University, Hyderabad, India, January 20-22, 2020, (MSSA-2020)entitled,
- i) Inhibitors of ISPH2 protein-An in silico study, by Pavithra M., Anusha J., Kiran Kumar M., Dheeraj Kumar S., **Vasavi, M.**
  - ii) Identification of novel lead molecules applying in silico studies for k1 protein by Madhavi Latha, B., Thirupathi, D., Vani, K., **Vasavi, M.**
  - iii) Insilico studies to identify novel lead molecules for DT1 protein targeting Tuberculosis by Thirupathi, D., Vani, K., Madhavi Latha, B., **Vasavi, M.**
  - iv) Interaction studies of target protein MB1, involved in triggering Tuberculosis - An insilico study by Anuradha, V., Lavanya, R., Mounika, B., **Vasavi, M.**
9. Presented a paper entitled "Identification of Novel Serpins as Inhibitors of SP1 Protein – An Insilico Approach" Kondaparthi Vani, Damera Thirupathi, Bingi Madhavalatha, Gangidi Priyadarshini and **Malkhed Vasavi**, at International conference on advances in chemical sciences and technologies organized by the Department of Chemistry, NIT Warangal, Telangana, INDIA during 23<sup>rd</sup> to 25<sup>th</sup> Sep 2019 (Best Poster Prize).

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10. Presented papers entitled below at International conference on emerging trends in spectroscopic techniques and their applications organized by Department of Chemistry, University College for Women, Koti, O.U, Hyderabad on 3<sup>rd</sup> and 4<sup>th</sup> Dec, 2018.
  - i) Advanced strategy for cancer treatment, insilico designing of photo sensitizer for dermatological applications”
  - ii) Method development and validation for estimation of Amlodipine besylate and perindopril argine tablet dosage –related impurities, by reverse phase ultra performance liquid chromatography
11. Identification of small molecular inhibitors for branched chain amino acid biosynthesis in Mycobacterium tuberculosis, Ramesh Malikanti, Rajender Vadija, Lavanya Rumandla, Kiran Kumar Mustayla, **Vasavi Malkhed**, Uma Vuruputuri\* presented at 20<sup>th</sup> International Conference of International Academy of Physical Science (CONIAPSXX) on Recent Advances in Physical Science and Future Challenges, organized by University College of Science, Osmania University, Hyderabad, during 14<sup>th</sup>-15<sup>th</sup> July 2017.
12. Attended International Conference on Drug Design: ICDD 2017 organized by Schrodinger llc at JNU Delhi on 7<sup>th</sup>-9<sup>th</sup> April 2017.
13. Homology modeling and Virtual screening studies to identify leads for MMT protein targeting Tuberculosis, Hymavathi Veeravarapu, Rajender Vadija, Ramesh Malikanti, **Vasavi Malkhed**, Lavanya R, Uma Vuruputuri\*, presented at an International Congress on Recent Advances in Chemistry And Chemical Engineering, organized by Department of Chemistry, JNTUH College of Engineering, Hyderabad (T.S.) India, during 11<sup>th</sup>-13<sup>th</sup> July 2016.
14. Identification of inhibitors for capsule glycogen biosynthesis in Mycobacterium tuberculosis by using In-Silico techniques, Lavanya Rumandla, Ramesh Malikanti, Hymavathi Veeravarapu, Rajender Vadija, Kiran Kumar Mustayla, **Vasavi Malkhed**, Uma Vuruputuri\*, presented at an International Congress on Recent Advances in Chemistry And Chemical Engineering, organized by Department of Chemistry, JNTUH College of Engineering, Hyderabad (T.S.) India, during 11<sup>th</sup> – 13<sup>th</sup> July 2016.
15. Identification of novel leads by applying *in silico* studies for *Mycobacterium tuberculosis* MR protein, Ramesh Malikanti, Rajendar Vadija, Kiran Kumar Mustayla, **Vasavi Malkhed**, Uma Vuruputuri\* presented at an international Conference and Workshop on Structure Based Drug Designing and Applications to infectious Diseases, at University of Hyderabad and IITH, Hyderabad, during 1<sup>st</sup>-5<sup>th</sup> February 2016
16. Homology modeling and Protein – Ligand docking studies of MR1 Protein, Ramesh Malikanti, Sravanthi Narani, U.S.H. Raghavendra Prasad, Rajender Vadija, Hymavathi Veeravarapu, Kiran Kumar Mustayla, **Vasavi Malkhed**, Uma Vuruputuri\* presented at an International conference on Trend Setting Innovation in Chemical Science & Technology– Applications in Pharma Industry (TSCST-API2015), organized by Centre for Chemical Sciences and Technology, Institute of Science and technology JNTUH, Hyderabad, during 16<sup>th</sup>-18<sup>th</sup> December 2015
17. Identification of novel leads by applying *in silico* studies for *Mycobacterium tuberculosis* MR2 protein, Ramesh Malikanti, Rajendar Vadija, Kiran Kumar Mustayla, **Vasavi Malkhed**, Uma Vuruputuri\*, presented at International Conference on biochemistry, nutrition &

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pharmacy in human welfare: recent trends and future challenges, organized by Department of Biochemistry, University College of Science, Osmania University, Hyderabad, during 3<sup>rd</sup> – 5<sup>th</sup> September 2015

18. Identification of PRL-2 inhibitors as novel antagonists for Cancer – An in silico approach, Lavanya Souda Padmarao, **Vasavi Malkhed**, Aboubakr H. Abdelmonsef, Thirupathi Dasari, Thirupathi Mukkera and Uma Vuruputuri\*, presented at the National conference in Bioinformatics and Drug discovery, Department of Botany, Nizam College, Basheerbagh, Hyderabad, India, during 22<sup>nd</sup>-24<sup>th</sup> December 2014
19. Insilico study of interaction of Ruthenium polypyridyl complexes with novel protein kinase, Navaneetha Nambigari, **Vasavi Malkhed** and Uma Vuruputuri\*, presented at the Indo-US conference on Molecular modeling and informatics in drug design, Organized by the Department of Medicinal Chemistry, National Institute of Pharmaceutical Education & Research (NIPER), Punjab, India, during 3<sup>rd</sup>-6<sup>th</sup> November-2014.
20. Transcriptional regulation of angiogenesis: A computational approach, Navaneetha Nambigari, **Vasavi Malkhed**, Rajender Vadeja and Uma Vuruputuri\*, presented at the International Conference on Chemical Biology Disease Mechanisms and Therapeutics (ICCB-2014), Organised by the Chemical Biology Society (IBS), India in association with CSIR- IICT, Tarnaka, Hyderabad, during 6<sup>th</sup> -8<sup>th</sup> February-2014.
21. In silico studies to identify novel lead molecules for VH1 targeting tuberculosis, Hymavathi Veeravarapu, Krishnaiah Dasari, Kiran Kumar M, **Vasavi Malkhed**, and Uma Vuruputuri\*, presented at the International Conference on Chemical Biology Disease Mechanisms and Therapeutics (ICCB-2014), Organised by the Chemical Biology Society (IBS), India in association with CSIR- IICT, Tarnaka, Hyderabad, during 6<sup>th</sup> -8<sup>th</sup> February-2014.
22. Pharmacophore mapping and 3D QSAR Studies of A1 Adenosine Receptor Kiran Kumar Mustyala, **Vasavi Malkhed**, Venkata Ramana Reddy Ch and Uma Vuruputuri\*, presented at the Conference on Recent Advances in computational Drug Design, Organised by the Indian Institute of Science, Bangalore and Schrödinger, during 16<sup>th</sup> – 17<sup>th</sup> September-2013.
23. In- Silico studies of novel TTF protein related to Mycobacterium tuberculosis. Kiran Kumar Mustyala, **Vasavi Malkhed**, Sarita Rajender Potlapally, Venkataramana Reddy. Ch. and Uma Vuruputuri\*, 3<sup>rd</sup> World Congress on Biotechnology 2012, organized by Omics group, at HICC, Hyderabad, India on 13-15 September, 2012.
24. Interaction Studies of Novel Antagonists for Tuberculosis-An Insilico Study, Anuradha Vippala, Kiran Kumar Mustyala, **Vasavi Malkhed**, Ramasree Dulapalli, Rajender Vadija, Uma Vuruputuri\*, 3<sup>rd</sup> World Congress on Biotechnology 2012, organized by Omics group, at HICC, Hyderabad, India on 13-15 September, 2012.
25. Presented a paper entitled “Identification of Novel potent inhibitors for S2 protein” Sarita Rajender Potlapally, **Vasavi Malkhed**, Ramasree Dulapalli, Bhargavi Kondagari, and Uma Vuruputuri\* at International Conference *UK-India MedChem 2011 Congress on Medicinal Chemistry* jointly Organized by Royal society of Chemistry, London, U.K. and IICT, Hyderabad, India (25<sup>th</sup> – 26<sup>th</sup> Feb 2011).
26. Presented a paper entitled “Homology modeling and docking study of human adenosine receptor A1” Phani G, Kiran Kumar M, Ramasree D, **Vasavi M**, Uma Vuruputuri\* in *4<sup>th</sup> International Symposium on Current trends in Drug discovery research* organized by Central Drug Research Institute, Lucknow, India (17<sup>th</sup> – 21<sup>st</sup> Feb, 2010).

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27. Participated in *IPS-USP 8<sup>th</sup> ASM 2009 Annual Scientific Meeting* organized by IPC- Indian Pharmacopoeia Commission and U.S. Pharmacopeia at Taj Krishna Hotel, Hyderabad, India (11<sup>th</sup> -12<sup>th</sup> Feb, 2009).
28. Presented a paper entitled Potent target for Cancer therapy, Sarita R, **Vasavi M**, Ramasree D, Uma Vuruputuri\* *Fourth Indo – US Lecture Series on Discrete Mathematical Chemistry* (With application to drug discovery, environmental protection, genomics and proteomics) jointly organized by Department of Chemistry, Nizam College (Autonomous), Osmania University, Hyderabad, India and Natural Resources Research Institute, University of Minnesota, Duluth, Minnesota – 55811, USA (6<sup>th</sup> – 9<sup>th</sup> Jan, 2009).
29. Presented Papers entitled Protein – Protein binding studies of TTK and ATRK, Bargavi G, Dheeraj Kumar S, **Vasavi M**, Uma Vuruputuri\* *Fourth Indo – US Lecture Series on Discrete Mathematical Chemistry* (With application to drug discovery, environmental protection, genomics and proteomics) jointly organized by Department of Chemistry, Nizam College (Autonomous), Osmania University, Hyderabad, India and Natural Resources Research Institute, University of Minnesota, Duluth, Minnesota – 55811, USA (6<sup>th</sup> – 9<sup>th</sup> Jan, 2009).
30. Presented a paper entitled “Multi – Pass Membrane Protein of *Mycobacterium tuberculosis* – 3DModel Assessment”, **Vasavi M**, Kalyan Chaitanya P, Uma Vuruputuri\*, in *Third Indo – US Lecture Series on Discrete Mathematical Chemistry* (with special reference to Chemoinformatics & Bioinformatics) jointly organized by The Department of Bioinformatics, School of Life Sciences Bharathidasan University, Tiruchirapalli, Tamilnadu and NRRI, Duluth, USA at Bharathidasan University, Tiruchirapalli, Tamilnadu, India (7<sup>th</sup> – 10<sup>th</sup> Jan, 2008).
31. Presented a paper entitled “Stress Gene Regulator Sigma J Model Evaluation and Binding Studies for Designing a New Drug” Kiran Kumar M, Swathi RP, **Vasavi M**, Kalyan Chaitnya P, Uma Vuruputuri\*, *DST- DFG Sponsored Indo-German Conference on Modeling Chemical and Biological [Re] activity* at ICT, Hyderabad, India (26<sup>th</sup> - 29<sup>th</sup> Sept, 2007).
32. Participated in *First Indo - US Lecture Series on Discrete Mathematical Chemistry*, jointly Sponsored by Indo-US Science and Technology Forum (IUSSTF) and DST held at PES Institute of Technology, Bangalore, India (8<sup>th</sup> -11<sup>th</sup> Jan,2007).
33. Presented a paper entitled QSAR Studies -Tricyclic Pthalimide analogues as Novel Inhibitors of HIV-1 Integrase, **Vasavi M**, Ramasree D, Sarita R, Uma Vuruputuri\*, in *International Symposium on Frontiers in Genetics and Biotechnology - Retrospect and Prospect*, Department of Genetics, Osmania University, Hyderabad, India (8<sup>th</sup> to 10<sup>th</sup> Jan, 2006).

## National Conferences

1. Presented a paper entitled “A DFT Study of Structural and Binding Properties of Cu (I) Polypyridyl Complexes with MMP - 2 Protein” at 25<sup>th</sup> CRSI National symposium in chemistry organized by IIT, Kanpur, U.P., INDIA during 19<sup>th</sup> – 21<sup>st</sup> Jul 2019.
2. Presented a paper entitled “Correlation of Electronic Structure and Antibacterial Activity of Ru (II) Polypyridyl Complexes: A DFT Approach” at 25<sup>th</sup> CRSI National symposium in chemistry organized by IIT, Kanpur, U.P., INDIA during 19<sup>th</sup> – 21<sup>st</sup> Jul 2019.

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3. Presented a paper entitled "Targeted therapy for cancer: An In silico approach" at Department of Physics, University College of Science, Saifabad, O.U., Hyderabad during 16<sup>th</sup> -17<sup>th</sup> Feb 2018.
4. Attended two day National seminar on Innovations and developments in emerging research trends in chemical science and technology, on 29<sup>th</sup> and 30<sup>th</sup> Dec, 2016
5. Participated in National Conference on Recent Advances in applied Nanomaterials organized by Department of Physics, University College of Science, Saifabad, Hyderabad during 4<sup>th</sup> – 5<sup>th</sup> March, 2016
6. Presented a poster entitled, Novel leads for inhibition of sulphate /thiosulphate ATP binding protein activity. Mounika Badineni, **Vasavi Malkhed**, Kiran Kumar Mustyala, Uma Vuruputuri\*, at ICC 2012, Dept. of Chemistry, Saurashtra University, Rajkot, Gujarat, India on 26<sup>th</sup> to 28<sup>th</sup> Dec 2012
7. Presented a paper entitled "Homology Modeling and Virtual Screening Studies of TKS2 protein of *Mycobacterium Tuberculosis*" Krishnaiah Dasari, Kiran Kumar Mustyala, **Vasavi Malkhed**, Sarita Rajender Potlapally and Uma Vuruputuri\* at ICC -XXX annual conference, Osmania University, Hyderabad, India (28<sup>th</sup>-30<sup>th</sup> December, 2011).
8. Presented a paper entitled "Comparative modeling and virtual screening of TTL Protein" Kiran Kumar M, **Vasavi M**, Bhargavi K, Sarita Rajender P, Uma Vuruputuri\* in *National Conference on biological Chemistry* organized by Gitam institute of science, Gitam University, Rushikonda, Vishakhapatnam, India (29<sup>th</sup> - 30<sup>th</sup> Nov, 2010).
9. Participated in *National Conference on Recent Advances in Chemical Research* at Department of Chemistry, Osmania University, Hyderabad, India (6<sup>th</sup> – 7<sup>th</sup> Feb, 2009).
10. Presented a paper entitled "Cell Membrane Protein Regulator Sigma F 3D Model Assessment and Binding Studies for Designing a New Drug", Neha Maria Isaac, **Vasavi M**, Kalyan Chaitanya P and Uma Vuruputuri\*, *National Symposium on Chemistry - Technology Interface A Synergistic Approach* at Nizam College, Hyderabad, India (30<sup>th</sup> Sept - 2<sup>nd</sup> Oct, 2007).
11. Presented a paper entitled Probable RNA Polymerase Sigma D factor - Evaluation of 3D Structure by Molecular Modeling Techniques Swati RP, Kiran Kumar M, Santosh K, **Vasavi M**, Uma Vuruputuri\*, in *National Symposium on Frontiers in Chemistry*, Dept of Chemistry, Kakatiya University, Warangal, Andhra Pradesh, India (23<sup>rd</sup> - 24<sup>th</sup> Feb, 2007).
12. UGC Sponsored National Symposium Organized by National Convention of Chemistry Teachers (NCCT) at the Department of Chemistry, Osmania University (Aug-2005).

### List of Conferences: Organising committee member

1. Organized (Convener) One-day Seminar on "**SPECTROSCOPIC ANALYSIS: IR, UV, NMR AND MASS SPECTROMETRY**" University College of Science, Saifabad, Osmania University, in collaboration with Royal Society of Chemistry, London, (Local Deccan Section), UK, on 05-08-2024. (Sponsored by Dean, Faculty of Sciences, OU, Hyderabad).
2. Organized (Organizing secretary) **1<sup>st</sup> International Conference on "Recent Innovations in Science and Technology"**. UCSS, OU, Hyderabad, Telangana, on 30-09-2023. (Sponsored by TSCHE, Hyderabad).

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3. Organising committee member of One-Day National Seminar On–**Organocatalysis: Prospects And Opportunities**, Department of Chemistry, University College of Science, Osmania University, Hyderabad, Telangana on 01-07-2023.
4. Organising committee member of **Current Trends and Futuristic Challenges in Chemical Sciences**, Department of Chemistry, UCS, Osmania University, Hyderabad, Telangana, India. During 29<sup>th</sup> – 30<sup>th</sup> Jul'2022.
5. Organising committee member of Webinar on “**Chemistry an affair with Academia and Industry**” Department of Chemistry, University College of Science, Saifabad, Osmania University, Hyderabad, Telangana on 08-09-2020.
6. Organising committee member of Webinar on “ **Interface of Academia and Industry in driving the Drug Discovery and development**” Department of Chemistry, University College of Science, Saifabad, Osmania University, Hyderabad, Telangana on 19-08-2020.
7. Organising committee member of “**Material Science for Societal Advancement 2020**”. Osmania University, Telangana, India. During 20<sup>th</sup> – 22<sup>nd</sup> Jan'2020.
8. Organizing Committee member of **20th International Conference of International Academy of Physical Science (CONIAPSXX) on Recent Advances in Physical Science and Future Challenges**, organized by University College of Science, Osmania University, Hyderabad, during 14<sup>th</sup> -15<sup>th</sup> July 2017.
9. Organizing Committee member of **Fourth Indo-US Lecture Series on Discrete Mathematical Chemistry** (With application to drug discovery, environmental protection, genomics, and proteomics) jointly organized by the Department of Chemistry, Nizam College (Autonomous), Osmania University, Hyderabad, India and Natural Resources Research Institute, University of Minnesota, Duluth, Minnesota – 55811, USA (6<sup>th</sup> – 9<sup>th</sup> Jan, 2009)
10. Organizing Committee member of **Futuristic Chemistry – 2007**, One-day Symposium organized by Dept of Chemistry, Nizam College, Hyderabad, India (8<sup>th</sup> Mar, 2007).
11. Participated in One-day seminar on **Drug Designing - An Insight Scope and Challenges**, at the Department of Chemistry, Nizam College, Hyderabad, India (20<sup>th</sup> July 2007).

### ANNEXURE – III

**Project Mentor** – Summer research projects for students from academic institutions.

- Sowmya Chivukula, 2022, Identification of New Lead Molecules against SWM1 and SWM2 Proteins for Cancer Therapy, Department of Chemistry, Osmania University, Hyderabad-500007, Telangana State, INDIA.
- Anusha J, 2020, Inhibitors of ISPH2 protein-An *in silico* study, Department of Chemistry, Loyola Academy, Old Alwal, Medchal, Hyderabad-500010, Telangana State, INDIA

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- Pavithra Macha, Identification of Inhibitors for MP1 protein – A Computational Approach, 2020, Department of Chemistry, Loyola Academy, Old Alwal, Medchal, Hyderabad-500010, Telangana State, INDIA
- May 2009, Homology and Docking studies of Adenosine Receptor – A1, Phani G, M.S. *Drug discovery, London University, London.*
- Aug 2009-Sep 2009, Comparative modeling and interaction studies of *Mycobacterium tuberculosis* protein –TBL, Shantkriti S, B.Tech Biotechnology, SRM University, Chennai.
- Apr 2008 - Jan 2009 3D modeling and Protein – Protein binding studies TTK and ATTK Bargavi G, M.Sc. *Organic Chemistry, O.U, Hyderabad.*
- May2007- Jun 2007 Cell Membrane Protein Regulator – TBF 3D Modeling studies Designing a New Drug Neha Isaac, B. Pharmacy, Malla Reddy Institute of Pharmaceutical Sciences, Jawaharlal Nehru Technological University, Hyderabad.
- Apr 2006 – Jun 2006 Probable RNAP subunit- Evaluation of 3D Structure. Swati RP, Kiran Kumar M and Santosh K M. Sc. *Chemistry, Nizam College, Osmania University, Hyderabad.*

### **Collaborations / Projects**

- ◆ Worked in collaboration with DST (Women Scientist Scheme - A), Dr. P. Sarita Rajender Nizam College, in “Novel targets for cancer therapy- Identification of new lead molecules” and (published 3 papers and 1 patent)
- ◆ Worked in collaboration with DST (Women Scientist Scheme - A), Ms. D. Ramasree, Nizam College; Project entitled “In Silico studies and identification of New Molecular Entities for novel apoptotic targets AT1 and AT2” (Published one article).
- ◆ Worked in collaboration with Ms. K. Bhargavi, Nizam College, New cancer therapeutics – Inhibitors for Novel Bcl-2 Mitochondrial protein to initiate apoptosis. (Published a paper)