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Date of Birth: 16th June 1980.

Marital Status: Married.

Wife: Mrs. Priya Rahul Jawarkar. (Msc. Mathematics. Bed, teacher at Dnyanmata High school, Irwin Square, Amravati)

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Rahul D. Jawarkar

Associate Professor, at Department of Pharmaceutical Chemistry, Dr. Rajendra Gode Institute of Pharmacy, University Mardi Road, Amravati.1/11/2020 to till date

Academic Credentials

PhD: Oriental University, Indore)
M-Pharmacy: Dr MGR Medical University Chennai.
PGDBM: Sant Gadge Baba Amravati university, Amravati.
B-Pharmacy: Government college of Pharmacy, Amravati
D-Pharmacy: Vidyabharati college of pharmacy, Amravati.

Experience (15+ Years)

1) Dr Rajendra Gode Institute of Pharmacy, University Mardi Road, Amravati, Maharashtra India Associate Professor from 1/11/2020 to present.
2) Adarsh College of Pharmacy, Vita, Sangili as Assistant Professor from 1/01/2015 to 30/10/2020.
3) P. Wadhwani College of Pharmacy, Yavatmal as Assistant Professor from 1/08/2012 to 11/08/2013 .
4) Sahyadri College of Pharmacy, Methwade, Sangola, Solapur district as Assistant Professor From 1/06/ 2011 to 31/07/2012.
5) Vidyabharati College of Pharmacy, Camp Road, Amravati as Assistant Professor From 1/07/2007 to 31/05/2011

Publications (Total Impact Factor: 240+)

1. Molecular docking, QSAR, and ADME studies of some pyrrolo [1, 2-a] benzimidazole-based quinones as novel topoisomerase 2 beta (TOP2β) inhibitors,RD Jawarkar, AN Khan, DR Bhagat, PN Khatale, PV Burakale, S Farooqui**, Chemical Physics Impact** 8, 100479 (IF:3.8).
2. QSAR modelling to predict structural features of certain sulfonamide as Urokinase-type Plasminogen Activator inhibitors RD Jawarkar, MEA Zaki, SA Al-Hussain, AYA Alzahrani, LC Ming, **Chemical Physics Impact** 8, 100544 (IF:3.8).
3. Structural, dynamic behaviour, in-vitro and computational investigations of Schiff's bases of 1, 3-diphenyl urea derivatives against SARS-CoV-2 spike protein S Ullah, A Ullah, M Waqas, SA Halim, AR Pasha, Z Shafiq, SN Mali, **Scientific Reports** 14 (1), 12588 (IF:3.8).
4. RP-HPLC Method Development and Validation of Rivaroxaban in Pharmaceutical Tablet Dosage Form T Bhatkar, P Burakle, P Ajmire, R Jawarkar, P Khatale, E Taywade, **Research Journal of Pharmacy and Technology** 17 (6), 2869-2874(IF:0.5).
5. Unveiling dynamics of nitrogen content and selected nitrogen heterocycles in thrombin inhibitors: a *ceteris paribus* approach VH Masand, S Al-Hussain, AY Alzahrani, AA Al-Mutairi, **Expert Opinion on Drug Discovery**, 1-19 (IF:6.5).
6. Multi-Target In-Silico modeling strategies to discover novel angiotensin converting enzyme and neprilysin dual inhibitors SK Shah, DD Chaple, VH Masand, RD Jawarkar, S Chaudhari, **Scientific Reports** 14 (1), 15991(IF:3.8).
7. Synthesis, biological evaluation, and molecular modelling of substituted thiazolyl thiourea derivatives: A new class of prolyl oligopeptidase inhibitors S Naseem, A Oneto, S Ullah, S Fatima, SN Mali, RD Jawarkar, A Khan, **International Journal of Biological Macromolecules** 275, 133571(IF:7.7)
8. Hydrazide–Hydrazones as Potential Antitubercular Agents: An Overview of the Literature (1999–2023) SN Mali, A Pandey, U Shah, RD Jawarkar, R Somani, **SynOpen** 8 (03), 173-184 (IF:2.75).
9. Multi-target in-silico modeling strategies to discover novel angiotensin converting enzyme and neprilysin dual inhibitors SK Shah, DR Chaple, VH Masand, RD Jawarkar, S Chaudhari, **Scientific reports** 14 (1), 20740(IF:3.8).

10. Cheminformatics Approaches to Predict the Bioactivity and to Discover the Pharmacophoric Traits Crucial to Block NF-κB RD Jawarkar, SN Mali, RG Ingle, SA Al-Hussain, AA Al-Mutairi, ...**Chemical Physics Impact**, 100720 (IF:3.8).
11. Synthesis, in silico studies and in vitro cytotoxicity evaluation of novel posaconazole derivative as a ALK TK inhibitor RD Jawarkar, P Sharma, S Jain, U Shah, MEA Zaki, SA Al-Hussain, **...Journal of Taibah University for Science** 18 (1), 2336674 (IF:3.8)
12. Theoretical and Experimental Investigations for Identification of Anaphylactic Lymphoma Kinase inhibitors, **Phys. Chem. Res**., Vol. 12, No. 3, 591-620, September 2024 DOI: 10.22036/pcr.2023.419100.2429 (IF:1.6,Q2) .
13. In silico study to recognize novel angiotensin-converting-enzyme-I inhibitors by 2D-QSAR and constraint-based molecular simulations. **Journal of Biomolecular Structure and Dynamics, 2023,** Impact factor:5.2.
14. Theoretical and Anti-Klebsiella pneumoniae Evaluations of Substituted 2, 7-dimethylimidazo [1, 2-a] pyridine-3-carboxamide and Imidazopyridine Hydrazide Derivatives. **Molecules, 2023, Impact factor:4.9.**
15. In-silico studies to recognize repurposing therapeutics toward arginase-I inhibitors as a potential onco-immunomodulators, **Frontiers in Pharmacology, 2023, Impact factor:5.9**
16. QSAR modeling approaches to identify a novel ACE2 inhibitor that selectively bind with the C and N terminals of the ectodomain, **Journal of Biomolecular Structure and Dynamics, 2023, Impact factor:5.2**
17. Synthesis, In-Silico, In Vitro and DFT Assessments of Substituted Imidazopyridine Derivatives as Potential Antimalarials Targeting Hemoglobin Degradation Pathway, **Journal of Computational Biophysics and Chemistry, Impact factor 2.2.**
18. **Rahul D Jawarkar,** R.L. Bakal, QSAR, Molecular Docking, MD Simulation and MMGBSA Calculations approaches to recognized concealed Pharmacophoric features requisite for the optimization of ALK Tyrosine kinase inhibitors as Anticancer leads, **published** in ***Molecules***, mdpi, **Manuscript no-1772266, (Impact factor 4.927)**
19. **Rahul D Jawarkar,** R.L. Bakal, Identification of hidden structural Features for the development of novel Anticancer leads as lysine-specific histone demethylase 1A (LSD1/KDM1A) inhibitor using QSAR, Molecular Docking, MD simulation and MMGBSA studies, **published** in ***Molecules***, mdpi, **Manuscript no-** 1793968**, (Impact factor 4.927)**
20. Ghosh A, Mukerjee N, Sharma B, Pant A, Kishore Mohanta Y, **Jawarkar Rahul D**, Bakal RL, Terefe EM, Batiha GE, Mostafa-Hedeab G, Aref Albezrah NK, Dey A, Baishya D. Target Specific Inhibition of Protein Tyrosine Kinase in Conjunction with Cancer and SARS-COV-2 by Olive Nutraceuticals. **Front Pharmacol**. 2022 Mar 8; 12:812565. Doi: 10.3389/fphar.2021.812565. PMID: 35356629; PMCID: PMC8959131 **(Impact Factor, 5.988, Frontiers).**
21. Bakal, R. L., **Jawarkar, Rahul D**., Manwar, J. V., Jaiswal, M. S., Ghosh, A., Gandhi, A., & Lewaa, I. (2022). Identification of potent aldose reductase inhibitors as antidiabetic (Anti-hyperglycemic) agents using QSAR based virtual Screening, molecular Docking, MD simulation and MMGBSA approaches. ***Saudi Pharmaceutical Journal***. **(Impact Factor-4.562, Elsevier**).
22. **Rahul D Jawarkar**, R.L. Bakal, Repurposing food molecules as a potential BACE1 inhibitor for Alzheimer's disease, **accepted** for publication in ***Frontiers in ageing Neuroscience*** **(Impact Factor, 5.702, Frontiers).**
23. Zaki MEA, Al-Hussain SA, Al-Mutairi AA, Masand VH, Samad A, **Jawarkar Rahul D**. Mechanistic Analysis of Chemically Diverse Bromodomain-4 Inhibitors Using Balanced QSAR Analysis and Supported by X-ray Resolved Crystal Structures. **Pharmaceuticals** (Basel). 2022 Jun 14;15 (6):745. Doi: 10.3390/ph15060745. PMID: 35745664; PMCID: PMC9231298. (**Impact factor-5.215, mdpi**).
24. Zaki, M.E.A.; Al-Hussain, S.A.; Al-Mutairi, A.A.; Masand, V.H.; Samad, A.; **Jawarkar, Rahul D**. Mechanistic Analysis of Chemically Diverse Bromodomain-4 Inhibitors Using Balanced QSAR Analysis and Supported by X-ray Resolved Crystal Structures. *Pharmaceuticals* **2022**, *15*, 745. https://doi.org/10.3390/ph15060745 (**Impact factor-5.215, mdpi)**.
25. Jain, C. M., Bakal, R. L., Burange, P. J., Kochar, N. I., Manwar, J. V**., Jawarkar, Rahul D**., & Lewaa, I. (2022). Exploring the use of herbal drugs and advanced supporting techniques for wound healing. ***Bulletin of the National Research Centre***, *46*(1), 1-17. **(Springer Nature).**
26. Manekar, S. S., Bakal, R. L., **Jawarkar, Rahul D**., & Charde, M. S. (2022). Challenges and measures during management of mounting biomedical waste in

COVID-19 pandemic: an Indian approach. ***Bulletin of the National Research Centre***, *46*(1), 1-9. **(Springer Nature).**

27. Chavhan, S.A., Bakal, R.L., **Jawarkar, Rahul D.** *et al*. Role of phytochemicals as potential radioprotectants. ***Bulletin of the National Research Centre*****,** 46, 48 (2022). https://doi.org/10.1186/s42269-022-00735-x **(Springer Nature).**

28. **R.D. Jawarkar**, R.L. Bakal, Magdi E.A. Zaki, Sami Al-Hussain, Arabinda Ghosh, Ajaykumar Gandhi, Nobendu Mukerjee, Abdul Samad, V.H. Masand, Israa Lewaa, QSAR Based Virtual screening derived Identification of a Novel Hit as a SARS CoV-229E 3CLpro Inhibitor: GA-MLR QSAR modeling supported by Molecular Docking, Molecular Dynamics Simulation and MMGBSA calculation Approaches, **Arabian Journal of Chemistry**, 2021, 103499, ISSN 1878-5352, https://doi.org/10.1016/j.arabjc.2021.103499. (**Impact Factor 6.212)**

29. Vijay H. Masand, Magdi E.A. Zaki, Sami A. Al-Hussain, Anis Ben Ghorbal, Siddhartha Akasapu, Israa Lewaa, Arabinda Ghosh, **Rahul D. Jawarkar**, Identification of concealed structural alerts using QSTR modeling for Pseudokirchneriella subcapitata, Aquatic Toxicology, Volume 239, 2021, 105962, ISSN 0166-445X, https://doi.org/10.1016/j.aquatox.2021.105962.(**Impact Factor -5.202)**

30. **Jawarkar, Rahul D**., Bakal, R. L., Khatale, P. N., Lewaa, I., Jain, C. M., Manwar, J. V., & Jaiswal, M. S. (2021). QSAR, pharmacophore modeling and molecular docking studies to identify structural alerts for some nitrogen heterocycles as dual inhibitor of telomerase reverse transcriptase and human telomeric G-quadruplex DNA. **Future Journal of Pharmaceutical Sciences**, *7*(1), 1-24**. (Springer Nature, IF: 2.6).**

31. Impact of tautomery of 3-(4H-1, 2, 4-triazol-3-ylthio)-N-phenylpropanamide on the COX-1 inhibitory mechanism. Published in **Journal of Enzyme inhibition and Medicinal Chemistry** February 5, 2012. (doi:10.3109/14756366.2011.654112) **(Impact factor 5.051**).

32. CoMSIA and POM analyses of anti-malarial activity of synthetic prodiginines, Bioorganic & Medicinal Chemistry Letters 22 (2012) 4827–4835 **(impact factor-2.94)**

33. Integrated GUSAR, QSAR and CoMFA analyses of Anti-malarial Activity of Natural and Synthetic Prodiginines for consensus pharmacophore identification published in **Journal of Chemical biology and drug design** (**impact factor 2.873**).

34. CoMSIA and POM analyses of anti-malarial activity of synthetic Prodiginines. Published in **Bioorganic and Medicinal chemistry letters,** Bioorganic & Medicinal Chemistry Letters 22 (2012) 4827–4835 (**Impact factor 2.94**).

35. BiS/MC algorithm based 3D-QSAR for receptor modelling to explore anti-malarial activity of synthetic prodiginines accepted for publication in **Chemometrics and Intelligent Laboratory Systems** DOI:10.29369/ijrbat.2014.02.i.0036 **(impact factor 4.175**).

36. Optimization of Antimalarial Activity of Synthetic Prodiginines: QSAR, GUSAR, and CoMFA analyses **Chem Biol Drug Des** 2013; 81: 527–536**(impact factor-2.873).**

37. QSAR and CoMFA studies of biphenyl analogs of the anti-tuberculosis drug (6S)-2-nitro-6-{[4-(trifluoromethoxy) benzyl]oxy}-6,7-dihydro-5H-imidazo[2,1-b][1,3]oxazine (PA-824), **Med Chem Res** (2012) 21:2624–2629**(Impact factor-2.351)**

38. k-NN, quantum mechanical and field similarity-based analysis of xanthone derivatives as a-glucosidase inhibitors, **Med Chem Res** (2012) 21:4523–4534, **(Impact factor-2.351)**

39. Molecular drug design, synthesis and pharmacophore site identification of Spiro heterocyclic compounds: Trypanosoma crusi inhibiting studies, Med Chem Res, **Med Chem Res**, DOI 10.1007/s00044-012-0010-5 **(Impact factor-2.351)**

40. Computational POM and 3D-QSAR evaluation of experimental in vitro HIV-1-Integrase inhibition of amide-containing diketoacids, **Med Chem Res** (2013) 22:1456–1464**(Impact factor-2.351).**

41. POM analyses of antitrypanosomal activity of 2-iminobenzimidazoles: favorable and unfavorable parameters for drugs optimization **Med Chem Res** (2013) 22:2437–2445**(impact factor-2.351)**

42. Molecular docking and quantitative structure–activity relationship (QSAR) analyses of indolylarylsulfones as HIV-1 non-nucleoside reverse transcriptase inhibitors, **Med Chem Res** (2014) 23:417–425(**impact factor-2.351)**

43. Does tautomerism influence the outcome of QSAR modeling? Med Chem Res (2014) 23:1742–1757**(impact factor-2.351)**

44. Synthesis and biological screening of 3-(N-substituted carboxamidomethylthio)-4-methyl-(4H)-1,2,4-triazoles**.** Indian Journal of Heterocyclic Chemistry 21(4):349-354**(impact factor-0.399)**
45. Design, synthesis of quinolinyl Schiff bases and azetidinones as enoyl ACP-reductase inhibitors, Medicinal Chemistry Research 24(11):1-20 DOI: 10.1007/s00044-015-1432-7**(impact factor-2.351)**
46. Synthesis and antimicrobial evaluation of 2-amino-6-[(5-pyridine-4-yl-1, 2, 4-triazole-4(H)-phenyl-3-ylthio) methyl]-4-substituted phenylnicotinonitriles published in **Indian Journal of Heterocyclic Chemistry.(Impact factor 0. 339)**
47. Synthesis and biological screening of 2-amino-3-cyano-6-[(5-pyridine-4-yl-1, 2, 4-triazole-4(H)-phenyl-3-yl-ethylthio) methyl]-4-substituted phenylnicotinonitriles. **Indian journal of Heterocyclic chemistry,** Vol 21, April-June, 2012,pp. 361-364 (**impact factor** 0. **339**)
48. Synthesis and Biological screening of 3-(N-substituted carboxamidomethylthio)-4-methyl-(4H)-1,2,4-triazoles, **Indian journal of Heterocyclic chemistry,** Vol 21, april-june,2012, pp. 349-354 (**impact factor** 0.**339**)
49. Computational POM and 3D-QSAR Evaluation of Experimental in vitro HIV-1 Integrase Inhibition of Amide-containing di-Ketoacids published in **Medicinal Chemistry Research (**in press) **(impact factor-2.351).**
50. 3D-QSAR Study on Coumarin Analogues as Potent Inhibitors of MAO-B using a COMFA Approach, Der Pharma Chemica, 2010, 2(6): 302-310
51. COMFA Analysis and toxicity risk assessment of coumarin analogues as Mao-A Inhibitors: Attempting better insight in drug design. Der Pharmacia Lettre, 2010, 2(6):350-357
52. 3D-QSAR studies on xanthone derivatives to understand pharmacological activities as MAO inhibitors, Der Pharma Chemica, 2010, 2(5): 22-32
53. Correlation potential of Wiener index vis-‡-vis molecular refractivity: Anti-malarial activity of xanthone derivatives, **organic chemistry: an Indian Journal**, OCAIJ, 6(1), 2010 [30-38]
54. Exploring interactions of 2-Amino-6-arylsulfonylbenzonitrile derivatives as non-nucleoside reverse transcriptase inhibitors of HIV-1 using docking studies, **J. Comput. Method. Mol. Design**, 2011, 1 (3): 39-48
55. Docking Studies of few C-3 Substituted Azapteridines as Hepatitis C Virus RNA-Dependent RNA Polymerase inhibitors, **J. Comput. Method. Mol. Design,** 2011, 1 (4):35-45
56. Experimental-Computational Evaluation of Antimicrobial Activity of Some β-Lactams: Advantages and limitations, **J. Comput. Method. Mol. Design**, 2011, 1 (4):28-34.
57. 8-POM as Efficient Tools to Predict and Improve Both Antibacterial and Antifungal Activity of Aryl Aldazines, **J. Comput. Method. Mol. Design**, 2011, 1 (3): 57-68 .
58. Investigating the interactions of FCS-304 and other Monoamine Oxidase (MAO) A Inhibitors Using Molecular Docking , **J. Comput. Method. Mol. Design**, 2011, 1 (3): 24-28 .
59. Presuming the Probable Anti-inflammatory Mechanism of Ursolic Acid: a plant derived pentacyclic triterpenoid, using molecular docking, **J. Comput. Method. Mol. Design,** 2011, 1 (2):9-13
60. Analysis of malathion in biological samples using thin layer chromatography, **BCAIJ**, 7(4), 2013 [141-144]
61. Synthesis, Biological Evaluation And Receptor Based Virtual Screening Of Novel 2 & 3-(4-Methyl-4h-1, 2, 4-Triazol-3-Ylsulfinyl)-N-Substituted Propanamide Derivatives As Selective Cox-2 Inhibitors Conference Paper. Aug 2012
62. RP-HPLC Method development and validation for the estimation of Duloxetine HCl enteric coated capsules. **International Journal of ChemTech Research**Vol.2, No.1, pp 239-241, Jan-Mar 2010.
63. Evaluation of antidiabetic activity of Caesalpinieabonduc (L.) roxb leaves (Caesalpiniaceae) in alloxan induced diabetic mice. **Indian J. Pharm. Educ. Res**. 43(3), Jul-Sept. 2009.
64. In-Vitro Evaluation of Antibacterial and Antifungal activity of Vitex Nirgundo (Verbenaceae). **Ethanobotanical Leaflets** 13:962-67, 2009.
65. Correlation potential of Wiener Index Vis-à-vis Molecular Refractivity: Antimalerial Activity of Xanthones Derivatives. **Organic Chemistry: an Indian Journal**, vol.6, issue 1, 2010.
66. Exploring the mechanism of Zanamivir as Anti-AIV agent by Molecular Docking and receptor based electrostatic analysis. **J. Comput. Method. Mol. Design**, 2011, 1 (1): 1-6.

67. Characterization, evaluation of products synthesized in the interaction of 4-(n-substituted)-3-pyridyl- 5- mercapto-s-triazole with secondary amines published in ***Der Pharma Chemica*****,**2011,3(5):334-340.
68. Identification of Pharmacophore and Anti-pharmacophore using GUSAR, QSAR and Molecular Docking. **Inventi Rapid: Molecular Modeling** Vol. 2011, Issue 4.
69. To investigate Mechanism of Dextrofloxacin-like antibiotics inhibits pneumococcal cell wall-degrading virulence factor. Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 1.
70. Synthesis and antimicrobial evaluation of 2-amino-6-[(5-pyridine-4-yl-1, 2, 4-triazole-4(H)-phenyl-3-ylthio) methyl]-4-substituted phenylnicotinonitriles published in **Indian Journal of Heterocyclic Chemistry.**
71. Molecular modeling studies on Odanacatib: a phase III clinical trial candidate for post-menopausal osteoporosis. published in Inventi **molecular modelling journal.**
72. Docking studies on 9-norbornylpurines as Coxsackievirus B3 inhibitor, Communicated to the Inventi **molecular modelling journal.**
73. Docking simulation studies on Spirodiketopiperazine-based CCR5 antagonist: an antiretroviral drug candidate. Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 1.
74. Modelling studies on novel benzopyran SC-75416 and SD-8381: a clinical trial candidate for selective cyclooxygenase-2 inhibition accepted for publication in Inventi **molecular modelling journal.**
75. Computational studies on Chalcone analogue from Glycyrrhiza inflata as novel influenza A (H1N1) neuraminidase. Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 1.
76. Molecular modeling analysis of INX-08189: A new clinical candidate for hepatitis C virus. Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 1.
77. To Envisage the Mechanism of L-735,524: P as HIV Protease-1 Inhibitor: a Phase 1 Clinical Trial Candidate. Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 1
78. To Envisage the Mechanism of L-735,524: P as HIV Protease-1 Inhibitor: a Phase 1 Clinical Trial Candidate. Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 1.
79. Design, Synthesis, Anti-inflammatory and Antioxidant activity: POM and Molecular Modeling Studies on Functionalized Flavonoids accepted for publication in **J. Comput. Method. Mol. Design**.
80. Characterization, evaluation of products synthesized in the interaction of 4- (N-substituted)-3-pyridyl- 5- mercapto-S-triazole with secondary amines, Published 2011, Chemistry
81. Comparative Account of Diverse Regulatory Guidelines for Storage and Transportation of Pharmaceuticals, IJPRIF, Vol.8, No.7, pp 180-192, 2015.
82. A Review: biological importance of mercapto substituted 1, 2, 4-triazole derivatives' on oxadiazole accepted for publication in **Research journal of pharmaceutical technology** (RJPT-1705).
83. A Review on biologically active mercapto 1, 3, 4-oxadiazole-2-thiol derivatives, **Asian Journal of research in chemistry,** 5(6): June, 2012 (AJRC-1223).
84. Docking analysis of Darunavir as HIV Protease inhibitors published in the Journal of Computational Methods in Molecular Design, 2012, 2 (1):39-43
85. Discovery of Novel Quinone Reductase 2 Inhibitor to Presume Binding Affinity and Inhibition using Molecular Docking Study, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4.
86. Discovery of Novel Quinone Reductase 2 Inhibitor to Presume Binding Affinity and Inhibition using Molecular Docking Study, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4.
87. Recognition of Lead Molecule as a Target for Phosphodiesterases Enzyme for the Treatment of Immune, Memory Related and Inflammatory Disorder, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4.
88. Discovery of Novel Scaffold (Zinc_982968) as Selective Cyclooxygenase 2 Inhibitor, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4
89. *In silico* Identification of Novel Inhibitor of Digestive Cathepsin L-Like Proteinases, Inventi Rapid: Molecular Modeling Vol. 2012, Issue 4.
90. Recognition of Novel Target for Monoamine Oxidase A (MAOA) Receptor, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4.
91. *In silico* Binding Analysis of Novel Lead for Targeting Caspase-6 Cysteine Protease for the Treatment of Alzheimer's and Huntington's Diseases, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4.
92. Discovery of Novel Acetylcholinesterase Inhibitor Implication for the Design of New Anti-Alzheimer Agents, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4.

93. Discovery of Novel Target for Phosphodiesterase (PDE4) Enzyme, Inventi Rapid: **Molecular Modeling** Vol. 2012, Issue 4.

Posters Presented

- Anticancer activity of *chloroxylon swetenia* in tumour induced swiss albino mice. *57th**IPC**, Hyderabad, 2006.*
- Antilice property of *Allium Cepa L.* against human head lice. ***Young Research conference**, IICT, Bombay 2008.*
- Separation of plant constituents from *Caesalpiniea bonduc (L.) roxb.* Leaves by HPTLC method. 59th, IPC, Banaras, 2009.
- Evaluation of antimicrobial activity of Caesalpiniea bonduc (L.) roxb. Leaves. 59th, IPC, Banaras, 2009.
- Evaluation of antidiarrhoeal activity of methanolic extract of Caesalpiniea coriaria (jacq) wild leaves. **Anant Pharma poster presentation, Pune** 2008
- Licicidal potential of Allium Cepa L. against human head lice. **International Herbal conference** 2009.Bangalore.
- QSAR studies on Antimalerial activity of new 4-amino-7-chloguinolyl amides, sulfonamides, ureas and thioureas. State level conference on "**Cheminformatic and Drug Discovery**" Poona College of arts, science and commerce, 2010.
- Exploring binding modes and structural features of 2-Amino-6-arylsulfonylbenzonitrile derivatives as non-nucleoside reverse transcriptase inhibitors of HIV-1. State level conference on "**Cheminformatic and Drug Discovery**" Poona College of arts, science and commerce, 2010.
- 3D QSAR studies on xanthone derivatives to understand pharmacological activities as MAO inhibitors. State level conference on "**Cheminformatic and Drug Discovery**" Poona College of arts, science and commerce, 2010.
- 3D QSAR studies on xanthone derivatives to understand pharmacological activities as MAO inhibitors. **Renacom**-2011; 29-30 April 2011/**Errachidia**, **Moroc.**
- Impact of coordination of stausporin to organometallic moiety on its antitumor activity: a model to understand pharmacological activities as kinase inhibitors. **Renacom**-2011; 29-30 April 2011/**Errachidia**, **Moroc.**
- 3D QSAR Studies on 2-aminobenzoxazole Derivatives as human peroxisome proliferator activated receptor (h) α agonists. Poster presented at AICTE sponsored National seminar on **Current trends in Molecular modelling in Drug design**, at pusad.2011.
- Docking Analysis of Darunavir as Hiv Protease Inhibitors. Poster presented at AICTE sponsored National seminar on **Current trends in Molecular modelling in Drug design**, at pusad. 2011.
- To probe Mechanism of Dextrofloxacin-like antibiotics inhibits pneumococcal cell wall-degrading virulence factor. Poster presented at AICTE sponsored National seminar on **Current trends in Molecular modelling in Drug design**, at pusad. 2011.
- Molecular Modeling Studies and Experimental Verification of Antibacterial Potential of a Series of some functionalized Flavonoids. Poster presented at AICTE sponsored National seminar on **Current trends in Molecular modelling in Drug design**, at pusad. 2011.
- Docking Studies of few C-3 Substituted Azapteridines as Hepatitis C Virus RNA-Dependent RNA Polymerase inhibitors. Poster presented at AICTE sponsored National seminar on **Current trends in Molecular modelling in Drug design**, at pusad. 2011.
- Docking studies on 9-norbornylpurines as Coxsackievirus B3 inhibitors. Poster presented at AICTE sponsored National seminar on **Current trends in Molecular modelling in Drug design**, at pusad. 2011.
- Development of CoMFA model for AZD4877analogues as Kinesin spindle protein inhibitors. Poster presented at 17th International conference on **expanding horizons in Chemical and Biological Sciences: Innovation crossroads**. ISCBC-2012 (21st -24th January,2012 Solapur)
- Probing the binding mode of Spirodiketopiperazine-based CCR5 antagonist: an antiretroviral drug candidate. Presented at**63rdIPC 2011 Bangalore.**
- Modeling studies on novel benzopyran SC-75416 and SD-8381: a clinical trial candidate for selective cyclooxygenase-2 inhibition. Presented at**63rd IPC 2011 Bangalore.**
- Docking studies on Chalcone analogue as novel influenza A (H1N1) neuraminidase inhibitors from Glycyrrhiza inflate. Presented at**63rdIPC 2011 Bangalore.**
- Molecular modeling studies on Odanacatib: a phase III clinical trial candidate for post-menopausal osteoporosis. Presented at **63rd IPC 2011 Bangalore.**

- Molecular modeling analysis of INX-08189: A new clinical candidate for hepatitis C virus. Presented at **63rd IPC 2011 Bangalore**
- To predict the mode of action of L-735,524: P as HIV protease-1 inhibitor: a phase 1 clinical trial candidate. Presented at **63rd IPC 2011 Bangalore.**
- In silico binding analysis of novel lead for targeting caspase-6 cysteine protease for the treatment of Alzheimer's and Huntington's diseases Presented at **64th IPC 2012,** Chennai.

Conferences \ Workshops Attended

- 57th **IPC**, Hyderabad, 2006.
- One Day seminar on '**Career opportunities in Clinical Research for Pharmacy'** held at Vidyabharti College of Pharmacy, Amravati.
- AICTE sponsored one day seminar on **Current trends in Molecular modelling in Drug design**, at pusad. 2011. (2nd Prize in poster presentation)
- Seventeenth International Conference on **'Expanding horizons in Chemical and Biological Sciences:** Innovation crossroads. ISCBC-2012 (21st -24th January,2012, Solapur)

Reviewer for

- Medicinal Chemistry Research (Springer Publisher)
- Bulletin of national research center (Springer Publisher)
- Heliyon (Cell Press)
- Computers in Biology & Medicine (Elsevier)
- Journal of Biomolecular structure and dynamics
- Molecules (MDPI, Publisher)
- Dove press Journal
- International journal of molecular science (MDPI, Publisher)
- Pharmaceuticals (MDPI, Publisher)
- Frontiers in Pharmacology (Frontiers Publisher)