PUBLICATIONS

Research Articles

1. Shaikh N, Sharma M and Garg P. An improved approach for predicting drug-target interaction: proteochemometrics to molecular docking. ***Molecular BioSystems*** 2016, **12:** 1006-1014.
2. Kumar R, Sethi R, Shah P, Roy I, Singh IP, Bharatam PV, Tewari R and Garg P. Biological Evaluation of Small Molecule Inhibitors of Mtb-ASADH Enzyme. ***Letters in Drug Design & Discovery*** 2016, **13:** 587-590.
3. Turakhiya A, Tangadpalliwar S, Sivakumar G, Amara VR, Tikoo K, Garg P and Bharatam PV. BiAnaCA: freely accessible pharmacoinformatics tool for data analysis of end-point biochemical assay. ***Journal of Bioinformatics, Computational and Systems Biology*** 2016, Accepted.
4. Rathod V, Belekar V, Garg P and Sangamwar AT. Classification of Human Pregnane x Receptor (hPXR) activators and non-activators by Machine learning techniques: A multifaceted Approach. ***Combinatorial Chemistry & High Throughput Screening*** 2016, **19:** 307-318.
5. Patil MD, Patel G, Surywanshi B, Shaikh N, Garg P, Chisti Y and Banerjee UC. Disruption of Pseudomonas putida by high pressure homogenization: a comparison of the predictive capacity of three process models for the efficient release of arginine deiminase. ***AMB Express*** 2016, Accepted.
6. Talluri MVNK, Kalariya PD, Dharavath S, Shaikh N, Garg P, Ramisetti NR and Srinivas R. Automated statistical experimental design approach for rapid separation of coenzyme Q10 and its biotechnological process related impurities using UPLC and UPLC/APCI/MS. ***Journal of Separation Science*** 2016, **39:** 3528-3535.
7. Swain D, Patel P, Gangam N, Sharma M, Garg P, Srinivas K and Samanthula G. Liquid Chromatographic Method Development for Forced Degradation Products of Dabigatran Etexilate: Characterisation and In Silico Toxicity Evaluation. ***Chromatographia*** 2016, **79:** 169-178.
8. Kumar R, **Garg P** and Bharatam PV. Pharmacoinformatics Analysis to Identify Inhibitors of Mtb-ASADH. ***Journal of Biomolecular Structure & Dynamics*** 2016, http://dx.doi.org/10.1080/07391102.2015.1005137.
9. Talluri MVNK, Kalariya PD, Reddy TJ, Sharma M, Garg P and Srinivas R. Characterization of stress degradation products of blonanserin by UPLC-QTOF-Tandem Mass Spectrometry. ***RSC Advances*** 2015, **85:** 69273-69288.
10. Talluri MVNK, Kalariya PD, Patel PN, P K, Sharma M, Garg P and Srinivas R. Rapid structural characterization of in vivo and in vitro metabolites of tinoridine

using UHPLC–QTOF–MS/MS and in silico toxicological screening of its metabolites. ***Journal of Mass Spectrometry*** 2015, **50:** 1222-1233.

11. Patel PN, Kalariya PD, Sharma M, Garg P, Talluri MVNK, Gananadhamu S and Srinivas R. Characterization of forced degradation products of pazopanib hydrochloride by UHPLC-Q-TOF/MS and *in silico* toxicity prediction. ***Journal of Mass Spectrometry*** 2015, **50:** 918-928.
12. Belekar V, Lingineni K and Garg P. Classification of Breast Cancer Resistant Protein (BCRP) Inhibitors and Non-inhibitors using Machine Learning Approaches. ***Combinatorial Chemistry & High Throughput Screening*** 2015, **18:** 476-485.
13. Kalariya PD, Sharma M, Garg P, Reddy TJ, Srinivas R and Talluri MVNK. Characterization of stress degradation products of mirabegron using UPLC-QTOF-MS/MS and *in silico* toxicity predictions of its degradation products. ***RSC Advances*** 2015, **5:** 31024-31038.
14. Rawat S, Gupta P, Kumar A, **Garg P**, Suri CR and Sahoo DK. Molecular mechanism of polyvinyl alcohol mediated prevention of aggregation and stabilization of insulin in nanoparticles. ***Molecular Pharmaceutics*** 2015, **12:** 1018-1030.
15. **Garg P**, Dhakne R and Belekar V. Role of Breast Cancer Resistance Protein (BCRP) as Active Efflux Transporter on Blood-Brain Barrier (BBB) Permeability. ***Molecular Diversity*** 2015, **19:** 163-172.
16. Khanapur S, Paul S, Shah A, Vatakuti S, Koole MJB, Zijlma R, Dierckx RAJO, Luurtsema G, **Garg P**, Waarde Av and Elsinga PH. Development of [18F]-labeled Pyrazolo[4,3-e]-1,2,4- triazolo[1,5-c]pyrimidine (SCH442416) analogs for the imaging of Cerebral Adenosine A2A receptors with Positron Emission Tomography. ***Journal of Medicinal Chemistry*** 2014 , **57:** 6765-6780.
17. Kumar R, Garg **P** and Bharatam PV. Shape-based virtual screening, docking and molecular dynamics simulations to identify Mtb-ASADH inhibitors. ***Journal of Biomolecular Structure & Dynamics*** 2014, , **33:** 1082-1093.
18. Kumar R, Sharma M, Shaikh N and Garg P. A comparative study of integrase binding domain of homologous HRP2 and LEDGF/p75 protein: From sequence to structural characterization. ***Molecular Simulation*** 2015, **41:** 683-690.
19. Negi A, Koul S, Gupta P, **Garg P** and Kumar R. Cystathionine • Lyase like Protein with Pyridoxal Binding Domain Characterized in Leishmania Major by Comparative Sequence Analysis and Homology Modelling. ***ISRN Computational Biology*** 2013, **2013:** Article ID 520435.

20. Sharma P, Kumar R, **Garg P** and Kaur J. Insights into Controlling role of Substitution Mutation, E315G on Thermostability of a lipase cloned from Metagenome of hot spring soil. ***3 Biotech*** 2014, **4:** 189-196.

21. Kumar R and **Garg P**. Molecular modeling and active site binding mode characterization of aspartate β-semialdehyde dehydrogenase family. ***Molecular Informatics*** 2013, **32:** 377-383.

22. Toor JS, Kumar R, **Garg P,** Sharma A and Arora SK. Prediction of High Level of Multiple Drug Resistance Mutations in HIV-1 Subtype C Reverse Transcriptase Gene among First Line Antiretroviral-Experienced Virological Failure Patients from North India Using Genotypic and Docking Analysis. ***Journal of AIDS and Clinical Research*** 2013, DOI: 10.4172/2155-6113.S5-005.

23. Belekar V, Shah A and **Garg P**. High Throughput Virtual Screening of Phloroglucinol Derivatives Against HIV-Reverse Transcriptase. ***Molecular Diversity*** 2013, **17:** 97-110.

24. Gupta P, **Garg P** and Roy N. In silico screening for identification of novel HIV-1 integrase inhibitors using QSAR and docking methodologies. ***Medicinal Chemistry Research*** 2013, **22:** 5014-5028.

25. Gupta P, Sharma A, **Garg P** and Roy N. QSAR study of curcumine derivatives as HIV-1 integrase inhibitors. ***Current Computer-Aided Drug Design*** 2013, **9:** 141-150.

26. Gupta P, **Garg P** and Roy N. Identification of novel HIV-1 integrase inhibitors using shape-based screening, QSAR and docking approach. ***Chemical Biology and Drug Design*** 2012, **79:** 835-849.

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33. **Garg P**, Sharma V, Chaudhari P and Roy N. SubCellProt: Predicting protein subcellular localization using machine learning approaches. ***In Silico Biology*** 2009, **9:** 35-44.

34. Gupta P, Roy N and **Garg P**. Docking-based 3D-QSAR study of HIV-1 integrase inhibitors. ***European Journal of Medicinal Chemistry*** 2009, **44:** 4276-4287.

35. Kaur S, Patel H, Sharma V, **Garg P** and Roy N. LeishBase: Leishmania major structural database. ***International Journal of Integrative Biology*** 2009, **7:** 63-68.

36. Gupta P and **Garg P**. Hypothetical models of *Leishmania major* proteins: a docking study of piperoyl amino acid derivative. ***Journal of Parasitic Diseases*** 2008 (Published in 2010), **32:** 123-127.

37. Agarwal A, Deswal S, Hanspers K and Conklin BR, **Garg P**, Roy N. Creation and validation of S. pombe gene database for GenMAPP analysis. ***International Journal of Integrative Biology*** 2007, **1:** 113-117.

38. Aher YD, Agarwal A, Bharatam PV and **Garg P**. 3D-QSAR studies of substituted 1-(3, 3-diphenylpropyl)-piperidinyl amides and ureas as CCR5 receptor antagonists. ***Journal of Molecular Modeling*** 2007, **13:** 519-529.

39. **Garg P** and Verma J. In silico prediction of blood brain barrier permeability: an Artificial Neural Network Model. ***Journal of Chemical Information and Modeling*** 2006, **46:** 289-297.

40. **Garg P** and Saxena SC. Prediction of Lipophilicity of Chemical Compounds Using Artificial Neural Network. ***EE-Pub,*** 2005.

Book Chapter

41. **Garg P**, Verma J and Roy N. In Silico Modeling for Blood Brain Barrier Permeability Predictions. In: Drug Absorption Studies - In Situ, In Vitro, and In Silico. Ehrhardt, Carsten; Kim, Kwang-Jin (Eds.). ***Springer, New York*** 2008, 510-556.

Review/General Article

42. Sharma M and Garg P. Computational Approaches for Enzyme Functional Class Prediction: A Review. ***Current Proteomics*** 2014, **11:** 17-22.
43. Agrawal A and **Garg P.** (2005) Applications of Artificial Neural Network in QSAR, CRIPS, 6, 12-16.

Report

44. Rao PR, Tiwari P, **Garg P**, Bansal P: **Impact of TRIPS on Pharmaceutical Prices.** 2006.

Databases/Software Developed

1. e-scider: A tool to retrieve, prioritize and analyze the articles from PubMed database, to Data Mining and Knowledge Discovery
2. BiAnaCA: freely accessible pharmacoinformatics tool for data analysis of end-point biochemical assay
3. MSubCellProt: Predicting multiple protein subcellular localization using machine learning approaches
4. SubCellProt: Predicting protein subcellular localization using machine learning approaches
5. TBIndia: Directory of R&D capabilities in the field of tuberculosis.
6. *Leish*Base: Leishmania major structural database.
7. ProIntPred: Protein-protein interaction prediction
8. GenMAPP database for fission yeast. A custom Gene Database and MAPP Archives for saccharomyces pombe have been created through collaboration with J. David Gladstone Institutes, at the University of California, San Francisco.
9. Label composition of all the formulations manufactured in India and their market value.
10. Pharmaceutical Education & Practicing Pharmacist Information System.
11. Software for predicting blood brain barrier permeability.
12. Central Animal Facility Management System (CAFMS).

Invited Lectures

1. **Garg P**. *Data mining and pattern recognition: Application to multi-target bioactivity prediction*. Molecular Modeling and Informatics in Drug Design. NIPER, S.A.S. Nagar. 2014

2. **Garg P**. *Data Mining and Pattern Recognition*. Computer Aided Drug Design: Hands-on Workshop. UIPS, Chandigarh. 2013
3. **Garg P**. *Data Base Management*. ITEC-2012, NIPER, S.A.S. Nagar. 2012
4. **Garg P.** Grid Computing for Bioinformatics/ Chemoinformatics Applications. In 5th India/Asean HyperWorks Technology Conference (HPC). Pune, India; 2009.
5. **Garg P**: Database Design & Pathways of Drug Metabolism. In SERC Summer School in Modeling and Informatics in Drug Design; S.A.S. Nagar. 2008
6. **Garg P**: Probabilistic Neural Network. In SERC Summer School in Modeling and Informatics in Drug Design; S.A.S. Nagar. 2008
7. **Garg P**. (2007). Artificial Neural Networks in Drug Discovery. Workshop on Pharmacoinformatics: Tools for Drug Target Identification, NIPER, S.A.S. Nagar, India.
8. **Garg P**. (2006). Drug Pricing Mechanism. Dissemination workshop on Impact of TRIPS on Pharmaceutical Prices, NIPER, S.A.S. Nagar, India.
9. **Garg P**. (2006). ANN in QSAR. Workshop on Pharmacoinformatics: QSAR, NIPER, S.A.S. Nagar, India.
10. **Garg P**. (2005). Artificial Neural Networks in Drug Discovery. Workshop on Pharmacoinformatics in drug design, NIPER, S.A.S. Nagar, India.
11. **Garg P**. (2004). Information Retrieval from Web: Techniques and Technologies. Workshop on Medicine Information. NIPER, S.A.S. Nagar, India.
12. **Garg P**. (2002). Electronic Information Retrieval (Computers for Enhanced Productivity). Training Program for Hospital Pharmacists of Himachal, NIPER, S.A.S. Nagar, India.

Conferences/Workshop/Abstract

1. Sonkusre S, Sharma M and Garg P (2016). Systems analysis of Klebsiella pneumoniae MGH 78578 metabolic model to identify potential drug targets. International Conference on System Biology (ICSB 2016). Barcelona.
2. Rathod V, Belekar V, Garg P and Sangamwar Abhay T (2016). Classification of Human Pregnane x Receptor (hPXR) activators and nonactivat ors by Machine learning techniques: A multifaceted Approach. QSAR 2016. USA.
3. Nimbalkar RD and **Garg P** (2016). Comparative conformational variation and flexibility analysis: Role of D-loop dynamics and its significance in the enzymatic activity of tankyrase inhibitors. Advances in Mathematical and Computational Biology (AMCB 2016). IIT Ropar, Punjab, India.

4. Sonkusre S, Sharma M and **Garg P** (2016). Systems analysis of Klebsiella pneumoniae MGH 78578 metabolic model to identify potential drug targets. Advances in Mathematical and Computational Biology (AMCB 2016). IIT Ropar, Punjab, India.
5. Nimbalkar RD and **Garg P** (2016). In Silico Alanine Scanning Mutagenesis of TNKS-TNKSI Complexes: Role of Computational Approaches in Molecular Recognition and Drug Design. Accelerating Biology 2016: Decoding the Deluge. C-DAC, Pune.
6. Shaikh N and **Garg P** (2015). A proteochemometrics based approach for therapeutic target prediction (P41). 11th German Conference on Chemoinformatics (GCC 2015), Fulda, Germany.
7. Kumar R, **Garg P** and Bharatam PV (2014). Structural characterization of Mtb-aspartate semialdehyde dehydrogenase active site to guide inhibitor design. Isolated Biomolecules and Biomolecular Interactions conference – IBBI 2014. Porquerolles Island.
8. Kumar R, Shaikh N, Sharma M and **Garg P** (2013). Sequence and Structural Homology Analysis of Integrase-Binding Domain in LEDGF and HDGFRP-2. National Conference on Recent Trends in Protein Structure Biology-2013 (NCRTPSB-2013), Jamia Millia Islamia, New Delhi, India.
9. Khanapur S, Paul S, Shah A, Zijlma R, Dierckx RAJO, **Garg P**, Waarde Av and Elsinga PH (2013). Development and Preclinical Evaluation of a Novel F-18 Labeled SCH442416 Analog for Imaging Adenosine A2A ReceptoEANM'13 - Annual Congress of the European Association of Nuclear Medicine, Lyon, France.
10. **Garg P**, Shah A, Kumar R and Sharma M (2013). "Pred-EC"- A Web Based Tool For Enzyme Functional Class Prediction. 3rd Indo-German Conference on Modeling Chemical and Biological (RE)Activity, NIPER, S.A.S. Nagar.
11. Naeem S, Shah A and **Garg P** (2013). A Systematic Prediction of Drug-Target Interactions by Machine Learning Approach. 3rd Indo-German Conference on Modeling Chemical and Biological (RE)Activity, NIPER, S.A.S. Nagar.
12. Patel N and **Garg P** (2013). Computational Modeling for TOR inhibitors using Machine Learning Approaches. 3rd Indo-German Conference on Modeling Chemical and Biological (RE)Activity, NIPER, S.A.S. Nagar.
13. Dhakne R and **Garg P** (2013). SVM based model for prediction of substrate and nonsubstrate of BCRP. 3rd Indo-German Conference on Modeling Chemical and Biological (RE)Activity, NIPER, S.A.S. Nagar.
14. Belekar V, Shah A and **Garg P** (2013). Prioritization of Phlororglucinol Derivatives against HIV Protease by Molecular Modeling Studies. 3rd Indo-

German Conference on Modeling Chemical and Biological (RE)Activity, NIPER, S.A.S. Nagar.

15. Kumar R and **Garg P**: *in silico* structural characterization of substrate analogue inhibitors binding mode for mycobac-terial aspartate • -semialdehyde dehydrogenase. 4th Seminar & Workshop on Computer Aided Drug Design. Puncak Alam, Malaysia. 2012
16. Gupta P, **Garg P**, Roy N: Identification of novel HIV-1 IN inhibitors by a shape based screening approach along with QSAR predictions and Docking studies. MipTec 2011, Congress Center Basel, Switzerland. 2011
17. **Garg P**, Sharma A, Kumar R, Gupta P, Roy N: MSubCellProt: Predicting Protein Multiple Subcellular Localization Using Machine Learning. In 3rd International Conference on Bioinformatics and Computational Biology (BICoB-2011), ISCA; March 23-25, 2011; New Orleans, Louisiana, USA. 2011
18. Mukherjee J, **Garg P**, Mittal A: e*Biochem*: A Web Based Bioinformatics & Life Science Job Management System for a HPC Cluster. In International Conference on Grid Computing and Applications (GCA 2010). Las Vegas, USA; 2010.
19. Gupta P, Roy N, **Garg P**: Identification of novel HIV-1 integrase inhibitors using shape-based screening and QSAR approach. In 18th European Symposium on Quantitative Structure-Activity Relationships; September 19-24, 2010; Rhodes, Greece. 2010
20. Gupta P, Roy N, **Garg P**: Docking, QSAR and shape-based screening of curcumine derivatives as HIV-1 integrase inhibitoIn International conference on Current Trends In Drug Discovery Research (CTDDR) CDRI, Lucknow, India; 2010.
21. **Garg P**: TBIndia: A Knowledge Support for Drug Discovery. In Seminar on Emerging Trends in the Diagnosis and Experimental Chemotherapy of Tuberculosis. NIPER, S.A.S. Nagar, India; 2009.
22. Dhindwal S, Sharma V, Roy N, **Garg P**: Protein-Protein Interaction Prediction and Network Mapping using Support Vector Machine. In International Conference on Open Source for Computer Aided Drug Discovery (OSCADD-2009). IMTECH, Chandigarh; 2009.
23. Gadhe CG, **Garg P**: Docking Directed CoMFA Study of Benzodithiazines Derivatives as HIV-1 Strand Transfer Integrase Inhibitors In International Conference on Open Source for Computer Aided Drug Discovery (OSCADD-2009). IMTECH, Chandigarh; 2009.
24. Gupta P, Roy N, **Garg P**: Docking studies of Tricylic HIV-1 Integrase inhibitors: Implication for two metal ions binding to the active site of integrase. In

International Conference on Open Source for Computer Aided Drug Discovery (OSCADD-2009). IMTECH, Chandigarh; 2009.

25. Patel H, Roy N, **Garg P**: A Comparison of Support Vector Machine And Probabilistic Neural Network As Multi-Class Classifiers For Protein Fold Recognition. In International Conference on Open Source for Computer Aided Drug Discovery (OSCADD-2009). IMTECH, Chandigarh; 2009.
26. Gupta P, Roy N, **Garg P**: Docking-based 3D-QSAR study of HIV-1 Integrase InhibitoIn International conference on New developments in drug discovery from natural products and traditional medicines (DDNP-TM). NIPER, S.A.S. Nagar; 2008.
27. Agrawal A, **Garg P**: CoMFA and CoMSIA 3D-QSAR Investigational Study of Piperidin-4-Carboxamide Derivatives as CCR5 Receptor Antagonists. In Bioinformatics and Drug Discovery; University of Hyderabad, Hyderabad, India.
28. Aher, Y.D. and **Garg P**. (2007) QSAR Modeling of CCR5 Receptor Antagonists using Artificial Neural Network, The IASTED Conference on Artificial Intelligence and Application, Innsbruck, Austria.
29. Sharma V, Roy N and Garg P (2007). Prediction of Enzyme Class of a Protein from Sequence Derived Features Using Artificial Intelligence. Workshop on Pharmacoinformatics: Tools for Drug Target Identification, NIPER, S.A.S. Nagar.
30. Sharma V, Chohan M, Garg P and Roy N (2007). Comparative Genomics Studies of Trypanomsomatid Parasitic Protozoa for Identification of Putative Targets. Workshop on Pharmacoinformatics: Tools for Drug Target Identification, NIPER, S.A.S. Nagar.
31. Chohan M, Sharma V, Garg P and Roy N (2007). Identification of Potential Targets in Plasmodium falciparum using Comparative Genomics. Workshop on Pharmacoinformatics: Tools for Drug Target Identification, NIPER, S.A.S. Nagar.
32. Aher Y and Garg P (2007). Artificial Neural Networks: Application to QSAR of CCR5 Receptor Antagonists. Workshop on Pharmacoinformatics: Tools for Drug Target Identification, NIPER, S.A.S. Nagar.
33. Gadhe C, Aher YD and Garg P (2007). ComFa and CoMSIA 3D-QSAR Investigations of Substituted N-[3-(4-benzylpiperidin-1-yl) propyl] N,N'-diphenylureas as CCR5 Receptor Antagonists. Workshop on Pharmacoinformatics: Tools for Drug Target Identification, NIPER, S.A.S. Nagar.
34. Garg D and Garg P (2006). Metabotox: A drug metabolism toxicity database. Workshop on Pharmacoinformatics: QSAR, NIPER, S.A.S. Nagar.

35. Agrawal A, Verma J and Garg P (2006). QSAR modeling of HIV-1 Integrase Inhibitors: An Artificial Neural Network Model. Workshop on Pharmacoinformatics: QSAR, NIPER, S.A.S. Nagar.
36. Wahajuddin, Garg P and Mohan CG (2006). In Silico Drug Discovery Endeavor for Drugs Acting on Angiotensin II Receptor. Workshop on Pharmacoinformatics: QSAR, NIPER, S.A.S. Nagar.
37. Agrawal A, **Garg P**: QSAR modeling of biological activity of HIV-1 inhibitors using Artificial Neural Network In Building Bridges, Forging Bonds for 21st Century Organic Chemistry and Chemical Biology; 7th-9th January 2006; NCL, Pune, India. ACS-CSIR Joint International Symposium 2006
38. Wahajuddin, **Garg P**, Mohan CG. (2006): *In silico* drug discovery endeavor for drugs acting on angiotensin II receptors In Building Bridges, Forging Bonds for 21st Century Organic Chemistry and Chemical Biology; 7th-9th January 2006; NCL, Pune, India. ACS-CSIR Joint International Symposium 2006
39. **Garg P**. (2005). Artificial Neural Network in Drug Discovery. IPSI - 2005 FRANCE, Carcassonne, France.
40. **Garg P**. and Saxena SC (2005). Prediction of ADME/T Properties of Drug/Drug Like Molecules Using Artificial Neural Network. National Conference on Recent Advances and Future Trends in IT, Patiala, Department of Computer Science, Punjabi University.

Research Guidance

Ph.D. students guided – 2 (completed); 4 (continuing)

M.S. (Pharm.) students guided – 31 (completed); 16 (continuing)

Projects

S.N.	Title	Funding Agency
1.	In silico prediction of blood brain barrier permeability using artificial intelligence.	DeitY, GOI
2.	In silico prediction of subcellular localization using artificial intelligence.	DeitY, GOI
3.	Directory of R&D capabilities in the field of Tuberculosis.	NSTMIS, DST, GOI
4.	Development of an in silico model for prediction of the HIV-1 integrase inhibitory activity and biological evaluation of the predicted molecules.	DBT, GOI

S.N.	**Title**	**Funding Agency**
5.	Practicing Pharmacists Information System	NSTMIS, DST, GOI.
6.	Development and Upgradation of Formulation Database	NPPA, GOI
7.	Impact of TRIPS on Pharmaceutical Prices.	MoHFW, GOI
8.	Development of packing norms	NPPA, GOI