

## PUBLICATIONS

### Research Articles

1. 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, Accepted.
2. Bodiwala HS, Sabde S, Gupta P, Mukherjee R, Kumar R, **Garg P**, Bhutani KK, Mitra D and Singh IP. Design and Synthesis of Caffeoyle-Anilides as Portmanteau Inhibitors of HIV-1 Integrase and CCR5. ***Bioorganic and Medicinal Chemistry*** 2011, **19**: 1256-1263.
3. Gupta P, **Garg P** and Roy N. Comparative docking and CoMFA analysis of curcumin derivatives as HIV-1 Integrase inhibitors. ***Molecular Diversity*** 2011, **15**: 733-750.
4. Toor JS, Sharma A, Kumar R, Gupta P, **Garg P** and Arora SK. Prediction of drug-resistance in HIV-1 Subtype C based on protease sequences from ART naive and first-line treatment failures in North India using genotypic and docking analysis. ***Antiviral Research*** 2011, (Accepted).
5. Gupta P, Kumar R, **Garg P** and Singh IP. Active site binding modes of dimeric phloroglucinols for HIV-1 reverse transcriptase, protease and integrase. ***Bioorganic and Medicinal Chemistry Letters*** 2010, **20**: 4427-4431.
6. Kumar R and **Garg P**. Active site binding interactions of  $\alpha$ -carboline derivative for HIV reverse transcriptase, protease and integrase. ***International Journal of Drug Discovery*** 2010, **2**: 51-55.
7. Singh IP, Jain SK, Kaur A, Singh S, Kumar R, **Garg P**, Sharma SS and Arora SK. Synthesis and Antileishmanial activity of Piperoyl-Amino Acid Conjugates. ***European Journal of Medicinal Chemistry*** 2010, **45**: 3439-3445.
8. **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.
9. 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.
10. 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.
11. 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.
12. 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.

13. Aher YD, Agarwal A, Bharatam PV and **Garg P**. 3D-QSAR studies of substituted 1-(3, 3-diphenylpropyl)-piperidiny l amides and ureas as CCR5 receptor antagonists. *Journal of Molecular Modeling* 2007, **13**: 519-529.
14. **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.
15. **Garg P** and Saxena SC. Prediction of Lipophilicity of Chemical Compounds Using Artificial Neural Network. *EE-Pub*, 2005.

#### **Book Chapter**

16. **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**

17. Agrawal A and **Garg P**. (2005) Applications of Artificial Neural Network in QSAR, CRIPS, 6, 12-16.

#### **Report**

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

#### **Databases/Software Developed**

1. ProIntPred: Protein-protein interaction prediction
2. MSubCellProt: Predicting multiple protein subcellular localization using machine learning approaches
3. SubCellProt: Predicting protein subcellular localization using machine learning approaches
4. Label composition of all the formulations manufactured in India and their market value.
5. LeishBase: Leishmania major structural database.
6. 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.
7. Pharmaceutical Education & Practicing Pharmacist Information System.
8. Directory of R&D capabilities in the field of tuberculosis.
9. Software for predicting blood brain barrier permeability.
10. Central Animal Facility Management System (CAFMS).

#### **Conferences/Workshop/Abstract**

1. 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
2. **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
3. Mukherjee J, **Garg P**, Mittal A: **eBiochem: 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.
4. 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
5. Gupta P, Roy N, Garg P: **Docking, QSAR and shape-based screening of curcumine derivatives as HIV-1 integrase inhibitors.** In International conference on Current Trends In Drug Discovery Research (CTDDR) CDRI, Lucknow, India; 2010.
6. Garg P: **Grid Computing for Bioinformatics/ Chemoinformatics Applications.** In 5th India/Asean HyperWorks Technology Conference (HPC). Pune, India; 2009.
7. Gupta P, Roy N, **Garg P**: **Docking studies of Tricyclic 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.
8. 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.
9. 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.
10. Gupta P, Roy N, **Garg P**: **Docking-based 3D-QSAR study of HIV-1 Integrase Inhibitors.** In International conference on New developments in drug discovery from natural products and traditional medicines (DDNP-TM). NIPER, S.A.S. Nagar; 2008.
11. **Garg P**: **Database Design & Pathways of Drug Metabolism.** In SERC Summer School in Modeling and Informatics in Drug Design; S.A.S. Nagar. 2008
12. **Garg P**: **Probabilistic Neural Network.** In SERC Summer School in Modeling and Informatics in Drug Design; S.A.S. Nagar. 2008
13. 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.

14. Agrawal A, **Garg P**: **QSAR modeling of biological activity of HIV-1 inhibitors using Artificial Neural Network** In Building Bridges, Forging Bonds for 21<sup>st</sup> Century Organic Chemistry and Chemical Biology; 7<sup>th</sup>-9<sup>th</sup> January 2006; NCL, Pune, India. ACS-CSIR Joint International Symposium 2006
15. Wahajuddin, **Garg P**, Mohan CG: **In silico drug discovery endeavor for drugs acting on angiotensin II receptors** In Building Bridges, Forging Bonds for 21<sup>st</sup> Century Organic Chemistry and Chemical Biology; 7<sup>th</sup>-9<sup>th</sup> January 2006; NCL, Pune, India. ACS-CSIR Joint International Symposium 2006
16. **Garg P.** (2005). Artificial Neural Network in Drug Discovery. IPSI - 2005 FRANCE, Carcassonne, France.
17. **Garg P.** (2005). Artificial Neural Networks in Drug Discovery. Workshop on pharmacoinformatics in drug design, NIPER, S.A.S. Nagar, India.
18. **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.
19. **Garg P.** (2004). Information Retrieval from Web: Techniques and Technologies. Workshop on Medicine Information. NIPER, S.A.S. Nagar, India.
20. **Garg P.** (2003). Electronic Information Retrieval. National Workshop on Curriculum Development in Natural Products at Postgraduate Level, NIPER, S.A.S. Nagar, India.
21. **Garg P.** (2002). Electronic Information Retrieval. Training Program for Hospital Pharmacists of Himachal, NIPER, S.A.S. Nagar, India.

### Projects

Funding agency	Title	Amount (Rs.)	Role
DIT	<i>In silico</i> prediction of subcellular localization	20,15,000/-	PI
DST	Directory of R&D capabilities in the field of Tuberculosis	19,91,512/-	PI
DBT	Development of <i>in silico</i> model for prediction of the HIV-1 integrase inhibitory activity and biological evaluation of the predicted molecules	20,74,400/-	Co-PI
DST	Pharmaceutical Education and practicing pharmacist information system	13,72,074/-	Co-PI
NPPA	Development of packing norms		Co-PI
NPPA	Label composition of all the formulations manufactured in India and their market value and updation of database		PI