

List of Published Research Papers/Reports/Reviews

29. Shikhar Gupta and **C Gopi Mohan***; 3D-Pharmacophore Model based Virtual Screening to Identify Dual-Binding Site and Selective Acetylcholinesterase Inhibitors. *Medicinal Chemistry Research*, (2010), (In press).
28. Jarvinen P, Fallarero A, Gupta S, **Mohan CG**, Hatakka A, and Vuorela P, Miniaturization and validation of the Ellmans reaction based acetylcholinesterase inhibitory assay into 384-well plate format and screening of a chemical library; *Combinatorial Chemistry and High Throughput Screening*, 2010 Mar;13(3):278-284.
27. Novel anti-inflammatory agents based on pyrazole based dimeric compounds; design, synthesis, docking and in vivo activity, Ashish K T, Priyanka S, Ved P S, Amit S, Goel RK, **Mohan C G**, *Bull. Chem. Soc. Japan*, (2010), (In press).
26. Vaibhav Jain, Ashish Pandey, Shikhar Gupta & **C Gopi Mohan***, Ligand-based molecular design of 4-benzylpiperidinealkylureas and amides as CCR3 antagonists, *Journal of Molecular Modelling*, 2010 Apr;16(4):669-676.
25. Jignesh Mungalpara, Ashish Pandey, Vaibhav Jain & **C Gopi Mohan***, Molecular Modeling and QSAR Analysis on Some Structurally Diverse N-type Calcium Channel Blockers, *Journal of Molecular Modelling*, 2010 Apr;16(4):629-644.
24. Mahendra Awale, Vivek Kumar, Saravanan P & **C Gopi Mohan***, Homology modeling and atomic level binding study of Leishmania MAPK with inhibitors, *Journal of Molecular Modelling*, 2010 Mar;16(3):475-488.
23. Ashish Pandey, Jignesh M & **C Gopi Mohan***, Comparative Molecular Field Analysis and Comparative Molecular Similarity Indices Analysis of Hydroxyethylamine Derivatives as Selective Human BACE-1 Inhibitor, *Molecular Diversity Journal*, 2010 Feb;14(1):39-49.
22. Adyary Fallarero, Päivi Oinonen, Shikhar Gupta, Pia Blom, Anna Galkin, **C. Gopi Mohan** & Pia M. Vuorela, Inhibition of acetylcholinesterase by coumarins: The case of coumarin 106, *Pharmacological Research*, Vol. 58, p(215-221), (2008).
21. **C Gopi Mohan*** & Tamanna Gandhi, Therapeutic Potential of Voltage Gated Calcium Channels, *Mini Review in Medicinal Chemistry*, Vol. 8(12), p(1285-1290), (2008).
20. Mahendra Awale & **C Gopi Mohan***, Molecular Docking Guided 3D-QSAR CoMFA Analysis of N-4-Pyrimidinyl-1H-indazol-4-amine Inhibitors of Leukocyte-specific protein tyrosine kinase. *Journal of Molecular Modelling*, Vol. 14(10), p(937-947), (2008).

19. Mahendra Awale & **C Gopi Mohan***, 3D QSAR CoMFA analysis of C5 substituted Pyrrolotriazines as HER2 (ErbB2) inhibitors; *Journal of Molecular Graphics and Modelling*, Vol. 26(7), p(1169-1178), (2008).
18. Divita Garg, Tamanna Gandhi & **C Gopi Mohan***, Exploring QSTR and Toxicophore of hERG K⁺ channel blockers using GFA and HypoGen techniques; *Journal of Molecular Graphics and Modelling*, Vol. 26 (6), p(966-976), (2008).
17. **C Gopi Mohan***, Tamanna Gandhi, Divita Garg, & Ranajit Shinde, Computer Assisted Methods in Chemical Toxicity Prediction; *Mini Review in Medicinal Chemistry*, Vol. 7 (5), p(499-507), (2007).
16. **C Gopi Mohan**, Investigational Drug Database (IDdb), Drug Report (2007), USA.
15. **C Gopi Mohan**, Thomson Pharma Report (2007), U.K.
14. Corradi HR, Corrigan AV, Boix E, **Mohan CG**, Sturrock ED, Meissner PN & Acharya KR, Crystal structure of protoporphyrinogen oxidase from *Myxococcus xanthus* and its complex with the inhibitor acifluorfen; *J Biol Chem*. Vol. 281(50): p(38625-38633), (2006), ACS, USA.
13. **C. Gopi Mohan**, Ester Boix, Hazel R. Evans, Zoran Nikolovski, M. V. Nogués, C.M. Cuchillo and K. Ravi Acharya, Crystal Structure of Eosinophil Cationic Protein in Complex with 2',5'-ADP at 2 Å Resolution reveals the details of the Ribonucleolytic Active site; *Biochemistry*, Vol.41(40), p(12100-6), (2002), ACS, USA.
12. **C. Gopi Mohan** and P.C. Mishra, Molecular Structure-Activity Relationship Study of Some Non-steroidal Anti-inflammatory agents using Electrostatic Potential Mapping; *Ind. J. Biochem. and Biophys*, Vol. 37, p(268-272), (2000), CSIR, India.
11. Anu K Moorthy, B. Gopal, **C. Gopi Mohan** and M.R.N. Murthy, Temperature dependent cell transformation in a Calcium-binding protein from *Entamoeba histolytica*; *Current Science*, Vol 77, No.7 (1999), India.
10. **C. Gopi Mohan** and P.C. Mishra, Electrostatic Potential Mapping using Hybridization Displacement Charge: Atomic Parameters and Transferability of Charge and Potential; *Int. J. Quantum Chemistry*, Vol. 66, p(149-156), (1998), John Wiley, USA.
9. **C. Gopi Mohan**, Anil Kumar and P.C. Mishra, Influence of Hybridization Displacement Charge on the Description of Electrostatic Potentials of Molecules with Multiple Electrophilic Sites; *Int. J. Quantum Chemistry*, Vol. 62, p(67-76), (1997), John Wiley, USA.
8. **C. Gopi Mohan** and P.C. Mishra, Electric Field Mapping and Structure-Activity Relationship for Cardiotonic Activities of Medorinone and Some of its Analogs; *Ind. J. Biochem. and Biophys*, Vol. 34, p(429-434), (1997), CSIR, India.

7. Anil Kumar, **C.G. Mohan** and P.C. Mishra, Molecular Electrostatic Potential and Field as Descriptors of Hydrogen Bonding and Molecular Activity. Effects of Hybridization Displacement Charge; J. Mol. Struct.(Theochem), Vol. 361, p(135-144), (1996), Elsevier, Netherlands.
6. **C. Gopi Mohan**, Anil Kumar and P.C. Mishra, An Optimized approach to Compute Hybridization Displacement Charge and a Study of its Effects on Electrostatic Potentials of Some Biologically Important Molecules; Int. J. Quantum Chemistry, Vol. 60, p(699-708), (1996), John Wiley, USA.
5. **C. Gopi Mohan**, Anil Kumar and P.C. Mishra, Effect of Optimized Hybridization Displacement Charge on the Description of Molecular Electrostatic Potentials of some Substituted Acetaldehydes; Proc. Ind. Acad. Sci. (Chem. Sci.), Vol. 108, p(469-484), (1996), India.
4. **C.G. Mohan**, Anil Kumar and P.C. Mishra, Electric Field Mapping and Structure-Activity Relationships for some Dihydropyridazinone Cardiotonics; J. Mol. Struct. (Theochem), Vol. 332, p(171-176), (1995), Elsevier, Netherlands.
3. Anil Kumar, **C.G. Mohan** and P.C. Mishra, Hybridization Displacement Charge in Molecules and its Effects on Electrostatic Potentials and Fields; Int. J. Quantum Chemistry, Vol. 55, p(53-60), (1995), John Wiley, USA.
2. **C.G. Mohan** and P.C. Mishra, Molecular Electric Field Mapping of Some Anions and Cations of 2-Aminopurine and 6-Thioguanine; Proc. Ind. Acad. Sci. (Chem. Sci.), Vol. 106, p(277-282), (1994), India.
1. **C.G. Mohan**, Anil Kumar and P.C. Mishra, Electric Field Mapping of some Anions and Cations of Adenine and Guanine; Int. J. Quantum Chemistry, Vol. 48, p(233-238), (1993), John Wiley, USA.

General/Popular articles

5. Tyagi, A., Gupta, S., and **Mohan, C. G.** *In silico* approach to discover multi-target-directed ligands for the treatment of Alzheimer's disease. In *Proceedings of the international Symposium on Biocomputing* (Calicut, Kerala, India, February 15 - 17, 2010). ISB '10. ACM, New York, NY, 1-8. DOI= <http://doi.acm.org/10.1145/1722024.1722032>.
4. N, Yogesh, P, Jignesh, K, Vivek, & **C Gopi Mohan**. Pharmacophore Modeling and Binding Analysis for targeting Mycobacterium tuberculosis MurC ligase . Available from Nature Precedings <<http://dx.doi.org/10.1038/npre.2010.4163.1>> (2010).

3. Patel, Jignesh, G, Gourja, Kumar, Vivek, Narkhede, Yogesh, Gupta, Shikhar, & **C. Gopi Mohan**. Homology Modeling of Human α_{2A} -Adrenoceptor . Available from Nature Precedings <<http://dx.doi.org/10.1038/npre.2009.4106.1>> (2009).
2. **C Gopi Mohan**, XML in Motion from Genome to Drug; Available from Nature Precedings < <http://dx.doi.org/10.1038/npre.2007.287.1> > (2007).
1. Ranjit Shinde, Divita Garg, Wahajuddin, & **C Gopi Mohan**, Impact of Structural Bioinformatics on Drug Discovery; Current Research & Information on Pharmaceutical Sciences, Vol. 6, No. 3, July-Sept., p(17-23), (2005).

Poster Publications in Conferences/Meetings:

27. Shikhar Gupta & **C. Gopi Mohan**, 3D-Pharmacophore Model based Virtual Screening to identify dual-binding site and Selective Acetylcholinesterase inhibitors, Current Trends in Drug Discovery Research (CTDDR-2010), 17-21st Feb. 2010, Organized by CDRI, Lucknow.
26. Ankit Tyagi, Shikhar Gupta & **C. Gopi Mohan**, *In Silico* Approach to Discover Multi-Target-Directed Ligands for the Treatment of Alzheimer's Disease. International Symposium on Biocomputing 2010, 15-17th Feb. 2010, Organized by Department of Biotechnology, National Institute of Technology, Calicut, Kerala.
25. Vivek Kumar, Shikhar Gupta, Gourja Gupta, Jignesh Patel & **C. Gopi Mohan**, Structure and Function Prediction of Human α_{2C} -Adrenoceptor Protein by Homology Modeling, Docking and Molecular Dynamics Simulation, Symposium on Recent Trends in Biophysics", and "Workshop on Emerging Techniques of Biophysics", from 13-16th Feb. 2010, Organized by Department of Physics, Banaras Hindu University, Varanasi. (**D.M. Bose Best Poster Award**)
24. N. Yogesh, P. Jignesh, K. Vivek, & **C.Gopi Mohan**, Pharmacophore Modeling and Binding Analysis for targeting Mycobacterium tuberculosis MurC ligase. 61st Indian Pharmaceutical Congress, Dec. 12-14, 2009, Nirma University, Ahmedabad.
23. Patel Jignesh, Narkhede Yogesh, Shikhar Gupta, & **C.Gopi Mohan**, Homology Modeling of Human α_{2A} -Adrenoceptor. 61st Indian Pharmaceutical Congress, Dec. 12-14, 2009, Nirma University, Ahmedabad.
22. V. Kumar, A. Arvind, M. Awale, **C Gopi Mohan**, An *In Silico* approach for Targeting HER2, 60th Indian Pharmaceutical Congress, Dec. 12-14, 2008.
21. **C Gopi Mohan** et. al. High-throughput *In vitro* screening and *In Silico* analysis to design Structurally Diverse AChE Inhibitors. International Conference on Drug Discovery from Natural Products and Traditional Medicines (DDNPTM-08) "New developments in drug

discovery from natural products and traditional medicines" from Nov. 16-20, 2008, NIPER, SAS Nagar, Punjab.

20. P. Saravanan and **C Gopi Mohan**, Alzheimer's Disease: From Genome to Drug, International Conference on Bioinformatics and Drug Discovery, Dec. 16-22, University of Hyderabad, 2007.
19. M. Jignesh, A Pandey and **C Gopi Mohan**, Structural Investigation of Dihydropyrazole Derivatives to design potent Inhibitors of Kinesin Spindle Protein. International Conference on Bioinformatics and Drug Discovery, Dec. 16-22, University of Hyderabad, 2007.
18. A Pandey, M. Jignesh and **C Gopi Mohan**, *In Silico* design of BACE Inhibitor for Alzheimer's disease, International Conference on Bioinformatics and Drug Discovery, Dec. 16-22, University of Hyderabad, 2007.
17. Tamanna Gandhi and **C Gopi Mohan**, *In silico* exploitation of T, International Conference on Chemoinformatics Jan 22-24, NCL, Pune, 2007.
16. S.V. Ronghe and **C. Gopi Mohan**, JAVATM based chemoinformatics tool with 3D interface and .NET support: MOLPHARM, International Conference on Chemoinformatics Jan 22-24, NCL, Pune, 2007.
15. **C Gopi Mohan** and Tamanna Gandhi, Identification of Selective T-type Calcium Channel Blockers, Abstract in Medicinal Chemistry Research, Vol. 15, Number 1/6, 2007.
14. Saravanan P and **C. Gopi Mohan**, Bioinformatics approach for the target identification for Alzheimer disease, Workshop on Pharmacoinformatics: Tools for drug target identification, 14-16th April, NIPER, 2007
13. Divita Garg and **C. Gopi Mohan**, *In silico* Model for Identifying HERG Inhibitors 10th International Conference on "Drug Discovery Perspectives and Challenges", Central Drug and Research Institute, February 24-25, 2006.
12. Ranajit Shinde and **C. Gopi Mohan**, 2D Quantitative Structure Activity Relationship for Prediction of P-glycoprotein Substrates and Non-substrates. 57th Indian Pharmaceutical Congress, Hyderabad, Dec. 2-4, 2005.
11. Wahajuddin, Garg P and **Mohan C. G.**, In silico Drug Discovery Endeavor for Drugs Acting on Angiotensin II Receptor. Joint International Conference on Advances in Organic Chemistry and Chemical Biology, ACS- CSIR Symposium, National Chemical Laboratory, Pune, January 6-9, 2006.
10. **C. Gopi Mohan**, Angélique Lagoutte, Benoît Guillot, Virginie Pischon- Pesme, Christian Jelsch and Claude Lecomte., Multipolar Refinement of High Resolution Crystal

Structure: Aldose Reductase and its Complexes. High Resolution Drug Design Meeting, 13-16th May, 2004, Bischenberg-Strasbourg, France.

9. Virginie Pischon- Pesme, Benoît Guillot, Angélique Lagoutte, **C Gopi Mohan**, Christian Jelsch and Claude Lecomte., Experimental Multipolar Charge Density Database used in Large Molecules Refinement. High Resolution Drug Design Meeting, 13-16th May, 2004, Bischenberg-Strasbourg, France.
8. Benoît Guillot, Christian Jelsch, Angélique Lagoutte, **Chethampadi Gopi Mohan**, Virginie Pichon-Pesme, Eric Chabriere and Claude Lecomte, s1.m3.p4 Charge Density Studies of Biological Macromolecules : beyond the Spherical Atom Model., 22nd European Crystallographic Meeting, ECM22, *Budapest, 2004 Acta Cryst.* (2004). **A60**, s116---- New methods for phasing, model building and real-time refinement
7. **C. Gopi Mohan**, Ester Boix, Hazel R. Evans, Zoran Nikolovski , M. V. Nogués, C.M. Cuchillo and K. Ravi Acharya., Crystal Structure of Eosinophil Cationic Protein in Complex with 2',5'-ADP at 2 Å Resolution. 6th International meeting on Ribonucleases, 19-23rd June, 2002, University of Bath, Bath, United Kingdom.
6. Participated in CCP4 meeting of the South West Structural Biology Consortium, 10-11th April, 2002, University of Exeter, Exeter, United Kingdom.
5. Participated in CCP4 Study Weekend "Highthroughput Structure Determination" 4-5th January, 2002, University of York, York, United Kingdom.
4. KR Acharya, GJ Swaminathan, E. Boix, **C Gopi Mohan**, Eosinophil 2001 International Symposium, Eosinophil Granule Proteins: Structural Insights into Functional Diversity, 4-8th May, 2001, Banff, Canada.
3. Participated in CCP4 Study Weekend "Molecular Replacement and its Relatives" 5-6th January, 2001, University of York, United Kingdom.
2. Participated in Frontiers in Structural Biology, 25-27th August 1999 and Protein Structural Bioinformatics and Genomics 28th August 1999, National Centre for Biological Sciences, Bangalore, India.
1. **C. Gopi Mohan**, Anil Kumar and P.C. Mishra, Drug Design through Analysis of Molecular Electrostatic Properties: Examples of Some Cardiotonic Drugs, National Symposium on Molecular and Cellular Biophysics and 23rd Annual Meeting of Indian Biophysical Society, 18-21st Feb, 1996, Department of Biophysics, All India Institute of Medical Sciences, New Delhi, India.

INVITED TALKS IN CONFERENCES/WORKSHOPS

12. 1st Refresher Course in Pharmacy held on 18th May, 2010, Pharmacy Department, Kurukshetra University, Haryana.
11. ITEC and SCCAP program held on 19-30th Oct. 2009, at NIPER, Mohali, Punjab.
10. Bioinformatics Orientation Training Cum Workshop held on 14-19th Sept. 2009, National JALMA Institute for Leprosy & Other Mycobacterial Diseases (ICMR), Agra.
9. Trend in Protein Modeling and Cheminformatics” 14-16th January, 2009, Institute of Microbial Technology, Chandigarh.
8. ITEC and SCCAP program held on 13-25th Oct. 2008, at NIPER, Mohali, Punjab.
7. SERC Summer School in Modeling and Informatics in Drug Design, 30-6-2008 to 18-7-2008.
6. Workshop on Pharmacoinformatics: Structure Based Drug Design, 13-15th April, 2008. (Sponsored by Department of Biotechnology and Pharma Industries), National Institute of Pharmaceutical Education & Research, Punjab.
5. MedChem-India Conference, Organizer: SELECT BIOSCIENCES Ld., Crestland House, Sudbury, CO10 OBD, U.K, Hyderabad, April 12-13, 2007.
4. Workshop on Pharmacoinformatics: Tools for Drug Target Identification, National Institute of Pharmaceutical Education & Research, Punjab, 14-16th March, 2007.
3. Lecture for UGC supported MSc. Bioinformatics course at Banaras Hindu University, Varanasi, 2007.
2. Workshop on “Pharmacoinformatics in Drug Design:QSAR”, National Institute of Pharmaceutical Education & Research, Punjab, 14-16th April, 2006.
1. Workshop on “Pharmacoinformatics in Drug Design”, National Institute of Pharmaceutical Education & Research, Punjab, 14-16th April, 2005.

Journal referee/reviewer:

1. Journal of Molecular Graphics & Modelling
2. Drug Discovery Today
3. QSAR and Combinatorial Science
4. European Journal of Medicinal Chemistry
5. Chemical Biology & Drug Design
6. Molecular Diversity
7. Indian Journal of Experimental Biology
8. Anti-infective agents in Medicinal Chemistry