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**PERMANENT ADDRESS:**

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INDIA

**WORKING ADDRESS:**

Assistant Professor  
Dept. of Pharmacoinformatics  
National Institute of Pharmaceutical  
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**PLACE AND BIRTH DATE**

Chennai,INDIA, FEBRUARY 13, 1966, Female

**NATIONALITY**

Citizen of India. Reside in India

**MARITUL STATUS**

Married

**PRESENT POSITION**

Assistant Professor, Department of  
Pharmacoinformatics, National Institute of  
Pharmaceutical Education and Research  
(NIPER), Sector 67, S. A. S. Nagar 160 062,  
India

**ACADEMIC QUALIFICATIONS:**

**Ph.D. (1992-1995) (Biophysics and Crystallography)** – Dept of Crystallography and Biophysics, University of Madras, Madras, Tamil Nadu. Thesis title:"STRUCTURAL AND CONFORMATIONAL STUDIES ON HOST-GUEST COMPLEXES".

**M.Phil.(1989-1990) (Biophysics)** – Dept. of Crystallography and Biophysics, University of Madras, Madras, Tamil Nadu.

**M.Sc. (1987 - 1989) (Biophysics)** – Dept. of Crystallography and Biophysics, University of Madras, Madras, Tamil Nadu.

**B.Sc. (1984-1987) (Physics) - S.D.N.B.**

Vaishnav College for Women, Madras, Tamil Nadu

**H.Sc. (Higher Secondary):** Christ King Girls Higher Secondary School, Tambaram, Madras, Tamil Nadu.

## **RESEARCH EXPERIENCE:**

### **Scientist at NIPER (1999-2004)**

Worked as scientist at Dept. of Medicinal Chemistry, NIPER

### **Research Associate at IMTECH (1997-1998)**

Worked on protein modeling and structure solution of macromolecules

### **Research Associate at Dept. of Biophysics, Delhi University South Campus (1995-1997)**

Molecular modeling studies of biologically important molecules.

## **COURSES TAKEN IN M.SC. & PH.D. PROGRAMMES:**

- Protein- Crystallography - Phase problem, Symmetries, Crystallization, Diffraction Techniques, Data collection, Electron density, Structure solution – Molecular replacement, Structure refinement
- Structural Biology – 3D structures of proteins and Macromolecules, Structure determination, Electron density map, Refinement of structures, Software packages, Application of structural information
- Computational Biology – Structures of proteins and biomolecules, Minimization techniques, Conformational search, Molecular mechanics and dynamics, Protein minimization, binding site and bioactive conformation
- Molecular Biophysics - Cell Biology- Bio Chemistry basis of gene action, Molecular structure of proteins, Nucleic acids and polysaccharides and Bio Molecular Assembly
- Bio-physical Techniques - Diffraction Methods, spectroscopy, NMR, ORD & CD, Electron Microscopy and other theoretical techniques
- Research Methodology – Numerical Methods, Statistical Methods and Computer Programming
- General Physics - Classical and Quantum Mechanics Statistical Mechanics - Thermodynamics- Electronics - Optics- Solid State Physics- Crystallography

- Mathematical Physics - Numerical Analysis - Laplacian Transformation - Probability Statistics - Trigonometry

## **CURRENT RESEARCH INTERESTS**

Rational drug design using CADD methods including 3D-QSAR, Molecular Docking, Receptor based and ligand based pharmacophore Mapping, Virtual Screening, Molecular Dynamics , *in silico* ADME and Toxicity prediction.

## **ONGOING PROJECTS:**

- Ligand and structure based design of active site and allosteric site directed PTP1B inhibitors
- Structural requirements for the design of selective and specific aldose reductase inhibitors
- Probing the Structural and Topological Requirements for CCR2 antagonism
- Ligand based and structure based design of Protein Kinase C (PKC) beta II–target for diabetic cardiomyopathy
- Computer aided design and molecular modelling studies on Enoyl reductase inhibitors as anti TB molecules
- *In silico* studies on neuramidase inhibitors

## **EXPERTISE:**

- Experienced in using other modeling and drug discovery software like Sybyl, Schrodinger, Discovery Studio, Open Eye. MoE, AMBER, Cerius2, Bio Suite, ADME Boxes, ALCHEMY, MOPAC, SPARTAN, GAUSSIAN.
- Gained working experience in SGI Power Onyx, Octane 2, FUEL, DEC alpha MVAX - VMS, VAX 730 Unix, Linux and MS - DOS environments.
- Familiar with packages like REFMAC (CCP4), SHELX-86, SHELX-76 and SDP that help in refinement and structure solution of proteins and small molecules.
- Gained experience in handling NONIUS – single crystal x-ray diffractometer.

## **RESEARCH GUIDANCE OFFERED**

### **Ph.D. students: 4 (ongoing)**

#### ***Title of the projects***

- Computer Aided Design of allosteric inhibitors of PTP1B, Ph.D.work pursued by Mr.Ranajit Shinde, from 2008.
- Molecular modeling studies on CCR2 and its antagonists, Ph.D. work pursued

by Mr. Rajesh Singh, from 2008.

- Molecular modeling studies on PKC $\beta$ 2, Ph.D. work pursued by Ms. Baljinder Kaur from 2008.
- Computer Aided Molecular Design of Enoylreductase Inhibitors as anti TB agents, Ph.D. work pursued by Mr. Vivek Kumar, from 2010.

**M.S. (Pharm.) students: 35**

**INVITED LECTURES DELIVERED: 30**

**NUMBER OF PRESENTATIONS IN CONFERENCES/SYMPOISUM: 40**

**LIST OF PUBLICATIONS:**

1. Dara Ajay and Sobhia ME. Identification of novel, less toxic PTP-LAR inhibitors using in silico strategies: pharmacophore modeling, ADMET-based virtual screening and docking. *Journal of Molecular Modeling* 2011 (In press).
2. Anup Shah and Sobhia ME. Induced fit binding of aldose reductase inhibitors. *Medicinal Chemistry Research*, 2011 (In Press).
3. Jain K and Sobhia ME. Targeting PKC- $\beta$  II by Peptides and peptidomimetics Derived from RACK 1: An *In Silico* Approach. *Molecular informatics* 2011, 30(1): 45-62.
4. Jain K, Ajay D, and Sobhia ME. Targeting PKC- $\beta$  II and PKB Connection: Design of Dual Inhibitors. *Molecular informatics* 2011. (In Press)
5. Chavan S, Kare P, Shah A, Hymavathi V and Singh R, Sobhia ME. MD studies on neuraminidase for probing binding pose of its inhibitors. *Medicinal Chemistry Research, Online First* 2010.
6. Divya PS, Jain K and Sobhia ME. From Peptides to Peptidomimetics: Design of PKC- $\beta$  II Inhibitors. *Chemical Biology and Drug Design* 2010.
7. Divya PS, Grewal BK and Sobhia ME. 2D and 3D QSAR analyses to predict favorable substitution sites in anilino monoindolyl maleimides acting as PKC $\beta$ II selective inhibitors. *Medicinal Chemistry Research, Online First* 2010.
8. Kumar R, Shinde R, Ajay D and Sobhia ME. Probing interaction requirements in PTP1B inhibitors: A Comparative Molecular Dynamics Study. *Journal of Chemical Informatics and Modeling* 2010, 50 (6): 1147-58.
9. Kumar H, Kumar R, Grewal BK and Sobhia ME. Insights into the Structural Requirements of PKC $\beta$ II Inhibitors Based on HQSAR and CoMSIA Analyses. *Chemical Biology and Drug Design* 2010, (In Press).
10. Sobhia ME and Singh R. Rational design of CCR2 antagonists: A survey of computational studies. *Expert Opinion in Drug Discovery* 2010, 5: 543-547.
11. Sobhia ME, Singh R, Kare P and Chavan S. De novo design of CCR2 antagonists: A survey of computational studies. *Expert Opinion in Drug Discovery* 2010, 5 (6): 543-557.

12. Singh R and Sobhia ME. Synergistic application of target structure-based alignment and 3D-QSAR study of protein tyrosine phosphatase 1B (PTP1B) inhibitors. *Medicinal Chemistry Research Online First* 2010.
13. Singh R and Sobhia ME. Homology modeling of human CCR2 receptor. *Medicinal Chemistry Research, Online First* 2010.
14. Kumar S, Chawla G, Sobhia M and Bansal AK. Characterization of solid-state forms of mebendazole. *Die Pharmazie* 2008, doi:10.1691/ph.2008.7168
15. Nair PC and Sobhia ME. Fingerprint directed scaffold hopping for identification of CCR2 antagonists. *Journal of Chemical Information and Modeling* 2008, 48 (9):1891-902.
16. Nair PC and Sobhia ME. Quantitative structure activity relationship studies on thiourea analogues as influenza virus neuraminidase inhibitors. *European Journal of Medicinal Chemistry* 2008, 43: 293-299.
17. Sobhia ME and Nair PC. Comparative QSTR studies for predicting mutagenicity of nitro compounds. *Journal of Molecular Graphics and Modeling* 2008 26(6) 916-934.
18. Sobhia ME, Nair PC and Srikanth K. QSAR studies on CCR2 antagonists with chiral sensitive hologram descriptors. *Bioorganic & Medicinal Chemistry Letters* 2008, doi:10.1016/j.bmcl.2008.01.023
19. Sobhia ME, Srikanth K and Nair PC. Probing the Structural and Topological Requirements for CCR2 antagonism: Holographic QSAR for indolopiperidine derivatives. *Bioorganic and Medicinal Chemistry Letters* 2008, 18: 1450-1456.
20. Sobhia ME and Nair PC. CoMFA based de novo design of pyridazine analogs as PTP1B inhibitors. *Journal of Molecular Graphics and Modeling* 2007 26(1):117-23.
21. Sobhia ME and Nair PC. Quantitative structure activity relationship studies on thiourea analogues as influenza virus neuraminidase inhibitors. *European Journal of Medicinal Chemistry* 2007, doi:10.1016/j.ejmech.2007.03.020.
22. Sobhia ME, Srikanth K and Nair PC. Probing the Structural and Topological Requirements for CCR2 antagonism: Holographic QSAR for indolopiperidine derivatives. *Bioorganic & Medicinal Chemistry Letters* doi: 10.1016/j.bmcl.2007.12.072.
23. Khurana J, Nair P and Sobhia ME. Design of Allosteric Ligands Using Computer Aided Drug Design (CADD) Techniques. *CRIPS* 2006.
24. Khanna S, Sobhia ME and Bharatam PV. Additivity of molecular fields: CoMFA study on dual activators of PPAR alpha and PPARgamma. *Journal of Medicinal Chemistry* 2005, 48, 3015.
25. Kumar S, Sobhia ME and Ramachandran U. L-Menthol as new scaffold for designing chiral phase-transfer catalysts. *Tetrahedron: Asymmetry* 16 2005, 2599-2605.

26. Thilagavathi R, Kumar R, Aparna V and Sobhia ME, Gopalakrishnan B, Chakraborti AK. Three-dimensional quantitative structure (3-D QSAR) activity relationship studies on imidazolyl and N-pyrrolyl heptenoates as 3-hydroxy-3-methylglutaryl-CoA reductase (HMGR) inhibitors by comparative molecular similarity indices analysis (CoMSIA). *Bioorganic & Medicinal Chemistry Letters* 2005 15(4):1027.
27. Sobhia ME and Bharatam PV. Comparative molecular similarity indices analysis (CoMSIA) studies of 1, 2-naphthoquinone derivatives as PTP1B inhibitors. *Bioorganic & Medicinal Chemistry* 2005, 13 (6), 2331.
28. Babu MA, Sobhia ME, Sharma M, Khanna S, Bharatam PV and Kaskhedikar SG. 3D-QSAR CoMFA CoMSIA studies on indomethacin derivatives as selective cyclooxygenase-2 inhibitors. *Indian Journal of Pharmaceutical Sciences* 2004, 66: 613-620.
29. Leto T, Sobhia ME and Bharatam PV. 3D-QSAR studies of pyruvate dehydrogenase kinase inhibitors based on a divide and conquer strategy. *Bioorganic & Medicinal Chemistry* 2004, 12 (10) 2709.
30. Chakraborti AK, Gopalakrishnan B, Sobhia ME and Malde A. Comparative molecular field analysis (CoMFA) of phthalazine derivatives as phosphodiesterase IV inhibitors. *Bioorganic & Medicinal Chemistry Letters* 2003, 13 (15) 2473.
31. Chakraborti AK, Gopalakrishnan B, Sobhia ME and Malde A. 3D-QSAR studies of indole derivatives as phosphodiesterase IV inhibitors. *European Journal of Medicinal Chemistry* 2003, 38 (11), 975.
32. Chakraborti AK, Gopalakrishnan B, Sobhia ME and Malde A. 3D-QSAR Studies on thieno [3, 2-d] pyrimidines as Phosphodiesterase IV Inhibitors. *Bioorganic Medicinal Chemistry Letters* 2003, 13 (8) 1403.
33. Kumar PS, Babu MK, Sobhia ME, Saxena AK and Kaskhedikar SG. 3D-QSAR Analysis of substituted 1, 3, 4-triaryl-3-pyrrolin-2-ones as selective cyclooxygenase-2-inhibitors. *Indian Journal of Pharmaceutical Sciences* 2003, 244.
34. Desiraju GR, Gopalakrishnan B, Jetty RKR, Nagaraju A, Sarma JARP, Sobhia ME and Thilagavathi R. Computer aided design of selective COX-2 inhibitors: Comparative Molecular Field Analysis, Comparative Molecular Similarity Indices Analysis and docking studies of some 1, 2-diarylimidazole derivatives. *Journal of Medicinal Chemistry* 2002, 45, 4847.
35. Desiraju GR, Sarma JARP, Raveendra D, Gopalakrishnan B, Thilagavathi R, Sobhia ME and Subramanya HS. Computer aided design of selective COX-2 inhibitors: comparative molecular field analysis and docking studies of some 3, 4-diaryloxazolone derivatives. *Journal of Physical Organic Chemistry* 2001, 4, 481.
36. Mande SC and Sobhia ME. Structural Characterization of protein-denaturant interactions: crystal structures of hen egg-white lysozyme in

complex with DMS and guanidinium chloride. *Protein Engineering* 2000, 13 (2)133.

**37.** Sobhia ME and Mande SC. Molecular Replacement. *News Letter in Macromolecular Crystallography* 1999, 1.

**38.** Sobhia ME, Chacko KK and Weber E. Crystal Structure of an Uncomplexed 25-Crown-7 comprising One 2, 6-Pyridino and Two 1, 4-Benzo Condensations. *Journal of Inclusion Phenomena and Molecular Recognition in Chemistry* 1994, 18, 1.

**39.** Ouchi, Araki T, Hakushi T, Sobhia ME, Chacko KK, Skobridis K and Weber E. Ring-Enlarged Dibenzo-Crown-6 Ethers. Cation Binding and X-ray Crystal Structure of Dibenzo-22-Crown-6.M. *Bulletin of the Chemical Society of Japan* 1993, 66, 2309.

**40.** Sobhia ME, Panneerselvam K, Chacko KK, Suh H, Weber E and Reutel C. Crystal Structure of the 2:1 complex of mercury (II) chloride with trithia pyridino 12-Crown-4 having unusual mercury co-ordination. *Inorganica Chimica Acta* 1992, 194, 93.

**41.** Panneerselvam K, Sobhia ME, Chacko KK, Weber E, Kohler H-J and Pollex R. Solid State Structure of the Hydrated Potassium Thiocyanate Complex of Benzo dinaphtho pyridino-21-Crown-7 C<sub>37</sub>H<sub>31</sub>NO<sub>6</sub>.KSCN (1:1:1). *Journal of Inclusion Phenomena and Molecular Recognition in Chemistry* 1992, 13, 29.