CURRICULUN VITAE

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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 Associate 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" under the guidance of Prof.K.K.Chacko.

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:

Associate Professor (July 201 2 – to date)

Working as Assisociate Professor at Dept. of Pharmacoinformatics, NIPER

Assistant Professor (July 2005 – June 2012)

Worked as Assistant Professor at Dept. of Pharmacoinformatics, NIPER

Scientist at NIPER (January 1999- June 2005)

Worked as scientist at Dept. of Medicinal Chemistry, NIPER

Research Associate at IMTECH (October1997-January 1999)

Worked on protein modeling and structure solution of macromolecules

Research Associate at Delhi University South Campus (July 1995- August 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 - Trignometry

PRESENT RESEARCH INTERESTS (in Computer Aided Molecular Design):

- Structure activity relationships using 3D-QSAR methods
- Pharmacophore mapping
- Homology modeling
- Molecular docking
- Identification of potential binding sites
- de novo ligand design
- Scoring functions
- Combinatorial library design
- Data base searching
- Virtual screening for lead selection and optimisation
- Optimization of lead compounds
- Quantum chemical methods
- Molecular mechanics and dynamics
- *in silico* ADME analysis
- Drug like and non-drug like molecules

OTHER RESEARCH AREAS OF INTEREST:

- Small molecular Crystallography
- Protein Crystallography

Ph.D. PROJECTS:

- Computational Approaches for The Rational Drug Design of Human Chemokine Receptor CCR2
- Molecular Modelling Studies for The Identification of Novel PTP1B Allosteric Inhibitors
- Molecular Modeling Studies for The Rational Design of Protein Kinase C –beta II Inhibitors
- Identification of Potential Direct Inha Inhibitors For Isoniazid- Resistant Tuberculosis: Insights From Computational Studies
- Molecular Modelling Studies on CD47 For Cancer
- Identification of Potential DNA-Gyrase Inhibitors as Anti Tuberculosis Agents
- Computer Aided Drug Design of HEX-2 Inhibitors in Cancer

FEW M.S. (Pharm.) PROJECTS COMPLETED AND ONGOING:

- Computer Aided Molecular Design of active site directed protein tyrosine phosphatase 1B inhibitors.
- Holographic QSAR study on active site directed PTP1B inhibitors.
- *De novo* ligand design of novel molecules for PTP1B using Leapfrog.
- Synergistic application of structure based and ligand based drug design for PTP1B.
- Design of less toxic molecules of the marketed diabetes drugs using informatics tools.
- Increasing the oral bioavailability of a few marketed drugs for diabetes, inflammation.
- Design of natural products based molecules as allosteric site PTP1B inhibitors.
- Virtual screening studies for CCR2 receptor for inflammation driven diseases.
- QSAR studies on CCR2 antagonists with chiral sensitive hologram descriptors.
- Probing the Structural and Topological Requirements for CCR2 antagonism: Holographic QSAR for indolopiperidine derivatives.
- Molecular docking studies on CCR2 antagonists for inflammation.
- Prediction of absorption of drugs using membrane QSAR.
- Development of QSTR models for carcinogens and mutagens.
- Study of multiple drug resistance (MDR) through P-gp.
- Ligand based and structure based design of Protein Kinase C (PKC) beta – target for diabetic cardiomyopathy.
- Computer-assisted Methods in Chemical Toxicity Prediction
- Pgp substrate and non-substrate prediction using Binary QSAR methodology.
- Structural requirements for the design of selective and specific aldose reductase inhibitors
- *In silico* studies on neuraminidase inhibitors

RESEARCH GUIDANCE OFFERED:

Ph.D. students: 7 (4 completed and 3 ongoing)
M.S. (Pharm.) students guided: >80
Number of current M.S.(Pharm.) students: 16

HONORS/AWARDS RECEIVED:

- Awarded DST – International travel grant to attend the International conference on Drug Discovery & Therapy World Congress, July 2015.

- Granted Bursary award to attend the Interanational Conference on CADD (**Joint eCheminfo - Innovation Well Autumn Community of Practice Meeting - Latest Advances in Drug Discovery Informatics)** October 2009, Philadelphia, PA, USA.

- Awarded full residential fellowship to attend 17th Residential School on Medicinal Chemistry, held at Drew University, Madison, New Jersey, June 2003.

- Invited to be a teaching faculty to conduct the workshop on "International Workshop on Drug Design," held at Birla Institute of Technology & Science, Pilani, Rajasthan, India.

- Awarded Department of Science and Technology's Fast Track Fellowship for Young Scientists for a period of three years (2005-2007) to work on research project entitled "Computer Aided Design Of Protein Tyrosine Phosphatase IB Ibhibitors (PTP1B) as Oral Anti Diabetic Agents".

- Awarded Council of Scientific and Industrial Research's Research Associate fellowship for a period of five year (Aug.'95-Aug. 2000) to carry out a project "CROWN ETHERS - AN EFFECTIVE ION CHANNEL" as a result of a project proposal submitted to CSIR's Science Programme under Life Sciences.

- Awarded Council of Scientific and Industrial Research's Senior Research Fellowship for a period of three years (Jan.'92 - Feb.'95) to carry out a project "STRUCTURAL AND STUDIES ON HOST - GUEST COMPLEXES" - as a result of a project proposal submitted to CSIR's Science Prog. Under Life Sciences.

DETAILS OF INTERNATIONAL CONFERENCES ATTENDED:

1.	Country visited:	**USA**
	Purpose:	To attend a school on medicinal chemistry and computer aided drug design
	Place and Date	Drew University, New Jersey, June 2003
2.	Country visited:	**UK**
	Purpose:	To attend an International conference on Computer Aided Drug Desgin (Virtual Discovery)
	Title of presentation	Identification of Novel CCR2 Scaffolds through Fingerprint Directed Virtual Screening
	Place and Date	London 23-25 October 2007
3.	Country visited	**USA**
	Purpose	To attend an International conference on "Latest advances on drug discovery and development"
	Title of presentation	Identification of selective and specific inhibitors for aldose reductase inhibitors using an *in silico* approach
	Place and Date	Philadelphia, October 12-16, 2009
4.	Country visited	**USA**
	Purpose	To attend International conference on DRUG DISCOVERY & THERAPY WORLD CONGRESS
	Title of presentation	Insights from molecular dynamics studies to combat isoniazid-resistant tuberculosis

Place and Date	July 22-25, 2015, Boston, MA.

RESEARCH GRANTS RECEIVED FROM EXTERNAL AGENCIES:

1. DST Project	
Title	Computer aided design of Protein Tyrosine Phosphata1B (PTP1B) Inhibitors as Oral Anti Diabetic Agents, funded by DST, (2005-2008).
Role	Principal Investigator
2. Industry project	Collaborative project between NIPER (CADD + Synthesis) and Torrent Research Centre, Ahemedabad (2008-2009)
Title	Design and synthesis of molecules for an important therapeutic target
Role	PI for Computer Aided Drug Design (CADD) Work
3. CSIR Project:	
Title:	Probing the mechanism and structureal requirements for CCR2 antagonism: Molecular Design of Novel, Potent and Small CCR2 antagonists for Inflammation Driven Research (2007-2011).
Role	Principal Investigator
4. CSIR Project:	
Title	Computer Aided Design of Selective and Specific aldose Reductas (ALR2) Inhibitors for Treatment of Diabetic Complications (2009-2011)
Role	Principal Investigator
5. DST Project	
Title	The challenges of new drug discovery for oral anti diabetic drugs: Molecular dynamics simulations, Pharmacophore modeling and Molecular design of PTP1B allosteric inhibitors (2014-2017)
Role	Principal Investigator
6. CSIR Project:	
Title	Studies on PTPIB allosteric inhibitors: In silico design, biological applications and protein crystallization (2014-2017)
Role	Principal Investigator

WORKSHOP/SYMPOSIUM CONDUCTED:

- One of the organizing Secretaries to conduct Workshop on Pharmacoinformatics: QSAR, March 2006, NIPER, Mohali.
- One of the organizing Secretaries to conduct Workshop on Pharmacoinformatics: Tools for target identification, March 2007
- One of the organizing Secretaries to conduct Workshop on Pharmacoinformatics: Structure Based Drug Design, March, 2008.
- Conducted one-day interactive workshop on OPENEYE software, Invited speaker: Dr.Paul Hawkins, Open Eye Scientific, USA, Feb. 2010.

FEW INTER INSTITUITIONAL PROJECTS:

Collaborating Institute	**Title of collaborative project**	**Type**	**Role**
International Sapient Discovery, LLC. 10929 San Diego, CA 92127. Sapient Drug Discovery	Design and Development of PTP1B inhibitors	Collaborative Project	PI for CADD work
IMTECH, Chanidgarh	Structure based design RIB-B inhibitors as anti bacterial agents	Collaborative Project	PI for CADD work
IIT-Chennai	Lead identifation and optimization for GABB-A receptor	Collaborative Project	PI for CADD work
IIT-Guwahati)	Design of CDK47 Inhibitors for Leukaemia	Collaborative Project	PI CADD work
University of Pretoria South Africa	DNA- gyrase inhibitors as anti tuberculosis agents	Collaborative Project	PI CADD work

EXPERTISE:

- Experienced in using other modeling and computational chemistry software Cerius2, MoE, AMBER, ADMET, MATLAB, BioSuite, ADME Boxes, ALCHEMY, MOPAC, SPARTAN, GAUSSIAN, CSD and ACDLABS.
- Gained working experience in SGI Power Onyx, Octane 2, FUEL, DEC alpha MVAX - VMS, VAX 730 Unix, Linux and MS - DOS environments.
- Acquired computer programming knowledge in FORTRAN.
- Experienced in the maintenance and up keeping of SGI machines.
- 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.

ADMINISTRATIVE EXPERIENCE:

- NIPER Girls Hostel Warden from 2014 – 2016
- Coordinated the workshop on Pharmacoinformatics :QSAR held in 2-5 March 2006.
- Served as the Chairman for Women Welfare Committee at NIPER
- Served as Senate member of NIPER
- Coordinated the work shop on Pharmacoinformatics in Drug Design held in 14-16 April 2005.
- Coordinated the work shop on Pharmacoinformatics in Drug Design held in 14-16 April 2005 (workshop brochure attached).
- Worked as Resident Tutor in the PG's Women's Gitanjali Hostel, University of Delhi South Campus from Nov.'96 to Feb.'97.
- Served as the chairman for Physical Verification of Equipments Committee in NIPER.

TRAINING OFFERED IN MOLECULAR MODELING:

M.Pharm. Students – >60

Ph.D. students /JRF- 10

SUPERVISED M.PHARM. PROJECTS: > 50

INVITED LECTURES DELIVERED (National): >30

NUMBER OF PRESENTATIONS IN CONFERENCES/SYMPOISUM : >50

REVIEWER FOR JOURNALS :BMCL, JCIM, BMC, JMM, EJMC, MCRE, MOLECULAR DIVERSITY, MOLECULAR SIMULATION, JMGM DRUG DISCOVERY LETTERS, JCAM, MedChemComm, ChemMedChem

RESEARCH PUBLICATIONS : 80

LIST OF PUBLICATIONS

1	Molecular dynamics-based investigation of InhA substrate binding loop for diverse biological activity of direct InhA inhibitors V Kumar, ME Sobhia Journal of Biomolecular Structure and Dynamics, 1-19	2016

2	Attenuation potential of rifampicin–phospholipid complex in murine hepatotoxicity model C Singh, LVSK Koduri, UA Kumar, TD Bhatt, V Kumar, ME Sobhia, ... Journal of Drug Delivery Science and Technology 30, 225-231	2015
3	Molecular Dynamics Assisted Mechanistic Study of Isoniazid-Resistance against Mycobacterium tuberculosis InhA V Kumar, ME Sobhia PloS one 10 (12), e0144635	2015
4	Inclusion complex of erlotinib with sulfobutyl ether-β-cyclodextrin: Preparation, characterization, in silico, in vitro and in vivo evaluation N Devasari, CP Dora, C Singh, SR Paidi, V Kumar, ME Sobhia, S Suresh Carbohydrate polymers 134, 547-556	2015
5	In silico identification of targets for a novel scaffold, 2-thiazolylimino-5-benzylidin-thiazolidin-4-one P Iyer, J Bolla, V Kumar, MS Gill, ME Sobhia Molecular diversity 19 (4), 855-870	2015
6	Molecular dynamics approach to probe PKCβII–ligand interactions and influence of crystal water molecules on these interactions BK Grewal, J Bhat, ME Sobhia Expert opinion on therapeutic targets 19 (1), 13-23	2015
7	2, 5-Diaryl-1, 3, 4-oxadiazoles as selective COX-2 inhibitors and anti-inflammatory agents J Grover, N Bhatt, V Kumar, NK Patel, BJ Gondaliya, ME Sobhia, ... RSC Advances 5 (56), 45535-45544	2015
8	Synthesis, biological evaluation and docking analysis of 3-methyl-1-phenylchromeno [4, 3-c] pyrazol-4 (1H)-ones as potential cyclooxygenase-2 (COX-2) inhibitors J Grover, V Kumar, ME Sobhia, SM Jachak Bioorganic & medicinal chemistry letters 24 (19), 4638-4642	2014
9	Leishmania donovani eukaryotic initiation factor 5A: Molecular characterization, localization and homology modelling studies S Singh, K Raju, D Jatekar, N Dinesh, MS Paul, ME Sobhia Microbial pathogenesis 73, 37-46	2014
10	Structural basis of conformational variance in phosphorylated and non-phosphorylated states of PKCβII BK Grewal, RV Krishnan, ME Sobhia Proteins: Structure, Function, and Bioinformatics 82 (7), 1332-1347	2014
11	Synthesis, biological evaluation, molecular docking and theoretical	2014

	evaluation of ADMET properties of nepodin and chrysophanol derivatives as potential cyclooxygenase (COX-1, COX-2) inhibitors J Grover, V Kumar, V Singh, K Bairwa, ME Sobhia, SM Jachak European journal of medicinal chemistry 80, 47-56	
12	Exploring a model of human chemokine receptor CCR2 in presence of TAK779: A membrane based molecular dynamics study A Balupuri, ME Sobhia Journal of Molecular Structure 1063, 131-138	2014
13	Insights into the bonding pattern for characterizing the open and closed state of the substrate-binding loop in Mycobacterium tuberculosis InhA V Kumar, ME Sobhia Future medicinal chemistry 6 (6), 605-616	2014
14	Essential gene identification and drug target prioritization in Leishmania species MLS Paul, A Kaur, A Geete, ME Sobhia Molecular BioSystems 10 (5), 1184-1195	2014
15	Digital holographic microscopy: a quantitative label-free microscopy technique for phenotypic screening B Rappaz, B Breton, E Shaffer, G Turcatti Combinatorial chemistry & high throughput screening 17 (1), 80-88	2014
16	Scaffold Hopping for Identification of Novel PKCβII Inhibitors Based on Ligand and Structural Approaches, Virtual Screening and Molecular Dynamics Study B K Grewal, M E Sobhia Combinatorial chemistry & high throughput screening 17 (1), 2-11	2014
17	Protein kinase C inhibitors: a patent review (2010–present) ME Sobhia, BK Grewal, MLS Paul, J Patel, A Kaur, T Haokip, A Kokkula Expert opinion on therapeutic patents 23 (11), 1451-1468	2013
18	Protein kinase C inhibitors: a patent review (2008–2009) ME Sobhia, BK Grewal, J Patel, A Kaur, T Haokip, A Kokkula Expert opinion on therapeutic patents 23 (10), 1297-1315	2013
19	Binding and discerning interactions of PTP1B allosteric inhibitors: novel insights from molecular dynamics simulations RN Shinde, ME Sobhia Journal of Molecular Graphics and Modelling 45, 98-110	2013
20	In silico design of peptidomimetics for PKC-β II inhibition: perspectives for diabetic cardiomyopathy therapy S Rohit, A Balupuri, ME Sobhia Medicinal Chemistry Research 22 (8), 3794-3801	2013

21	Structure prediction and molecular dynamics simulations of a G-protein coupled receptor: human CCR2 receptor R Singh, ME Sobhia Journal of Biomolecular Structure and Dynamics 31 (7), 694-715	2013
22	The following is a list of selected recently published Expert Opinion articles, related to the content of this issue of Expert Opinion on Therapeutic Patents Nutraceuticals for prostate cancer chemoprevention: from molecular mechanisms to clinical application Z Wang, J Fan, M Liu, S Yeung, A Chang, MSS Chow, D Pon, Y Huang, ... Therapy 17 (3), 281-291	2013
23	Structure-based design and analysis of MAO-B inhibitors for Parkinson's disease: using in silico approaches P Kare, J Bhat, ME Sobhia Molecular diversity 17 (1), 111-122	2013
24	From peptides to peptidomimetics: rational design of potential PKC-β II inhibitors PS Divya, K Jain, ME Sobhia Medicinal Chemistry Research 22 (2), 625-634	2013
25	The following is a list of selected recently published Expert Opinion and Expert P Gambadauro, ME Sobhia, BK Grewal, MLS Paul, J Patel, A Kaur, ... Matrix 54 (1), 145-152	2013
26	Characterisation of the flexibility of substrate binding loop in the binding of direct InhA inhibitors V Kumar, ME Sobhia International journal of computational biology and drug design 6 (4), 318-342	2013
27	Development of 3D-pharmacophore model followed by successive virtual screening, molecular docking and ADME studies for the design of potent CCR2 antagonists for inflammation-driven diseases R Singh, A Balupuri, ME Sobhia Molecular Simulation 39 (1), 49-58	2013
28	Antibody Targated Theraphy: Application Towards Cancer and Viral Diseases. Tumbhi K.,Ankit G., Thapaswini P., Venkat KR., Sobhia M.E.,CRIPS13(3)., 2012	2012
29	Theoretical investigations on maleimide and its indolyl derivatives: Rational drug design approach for PKCβII inhibitors BK Grewal, ME Sobhia Journal of Molecular Structure 1029, 35-44	2012

30	In silico identification of novel PKC βII inhibitors: ligand and receptor based pharmacophore modeling, virtual screening, and molecular dynamics study BK Grewal, ME Sobhia Journal of Cheminformatics 4, 1-1	2012
31	Identification of specific features of inhibition of PKCβII and its potential lead by shape-based virtual screening and molecular docking studies BK Grewal, ME Sobhia Bioorganic & medicinal chemistry letters 22 (14), 4672-4677	2012
32	Induced fit binding of aldose reductase inhibitors to AKR1B10 A Shah, R Shinde, P Kare, V Hymavathi, S Chavan, ME Sobhia Medicinal Chemistry Research 21 (7), 1245-1252	2012
33	Geometrical criteria for characterizing open and closed states of WPD-loop in PTP1B RN Shinde, ME Sobhia Journal of Molecular Structure 1017, 79-83	2012
34	Binding site characterization of G protein-coupled receptor by alanine-scanning mutagenesis using molecular dynamics and binding free energy approach: application to CC chemokine receptor-2 (CCR2) S Chavan, S Pawar, R Singh, ME Sobhia Molecular diversity 16 (2), 401-413	2012
35	Novel insights into the structural requirements for the design of selective and specific aldose reductase inhibitors H Kumar, A Shah, ME Sobhia Journal of molecular modeling 18 (5), 1791-1799	2012
36	Stereoselective synthesis of sugar-based β-lactam derivatives: docking studies and its biological evaluation S Nagarajan, P Arjun, N Raaman, A Shah, ME Sobhia, TM Das Tetrahedron 68 (14), 3037-3045	2012
37	Insights into the permeability of drugs and drug-likemolecules from MI-QSAR and HQSAR studies RN Shinde, K Srikanth, ME Sobhia Journal of molecular modeling 18 (3), 947-962	2012
38	Protein kinase C βII in diabetic complications: survey of structural, biological and computational studies ME Sobhia, BK Grewal, J Bhat, S Rohit, V Punia Expert opinion on therapeutic targets 16 (3), 325-344	2012
39	Protein tyrosine phosphatase inhibitors: a patent review (2002–2011) ME Sobhia, S Paul, R Shinde, M Potluri, V Gundam, A Kaur, T	2012

	Haokip Expert opinion on therapeutic patents 22 (2), 125-153	
40	Identification of novel, less toxic PTP-LAR inhibitors using in silico strategies: pharmacophore modeling, SADMET-based virtual screening and docking D Ajay, ME Sobhia Journal of molecular modeling 18 (1), 187-201	2012
41	MD studies on neuraminidase for probing binding pose of its inhibitors S Chavan, P Kare, A Shah, V Hymavathi, R Singh, ME Sobhia Medicinal Chemistry Research 20 (9), 1680-1686	2011
42	Homology modeling of human CCR2 receptor R Singh, ME Sobhia Medicinal Chemistry Research 20 (9), 1704-1712	2011
43	Molecular dynamics directed CoMFA studies on carbocyclic neuraminidase inhibitors S Chavan, S Bhayye, ME Sobhia Molecular diversity 15 (4), 979-987	2011
44	2D and 3D QSAR analyses to predict favorable substitution sites in anilino-monoindolylmaleimides acting as PKCβII selective inhibitors PS Divya, BK Grewal, ME Sobhia Medicinal Chemistry Research 20 (8), 1188-1199	2011
45	Simplified Receptor Based Pharmacophore Approach to Retrieve Potent PTP-LAR Inhibitors Using Apoenzyme D Ajay, ME Sobhia Current computer-aided drug design 7 (3), 159-172	2011
46	Insights into the Structural Requirements of PKCβII Inhibitors Based on HQSAR and CoMSIA Analyses H Kumar, R Kumar, BK Grewal, ME Sobhia Chemical biology & drug design 78 (2), 283-288	2011
47	Synergistic application of target structure-based alignment and 3D-QSAR study of protein tyrosine phosphatase 1B (PTP1B) inhibitors R Singh, ME Sobhia Medicinal Chemistry Research 20 (6), 714-725	2011
48	Targeting PKC-β II and PKB Connection: Design of Dual Inhibitors K Jain, D Ajay, ME Sobhia Molecular informatics 30 (4), 329-344	2011
49	Targeting PKC-β II by Peptides and Peptidomimetics Derived from RACK 1: An In Silico Approach K Jain, ME Sobhia	2011

	Molecular Informatics 30 (1), 45-62	
50	Rational design of CCR2 antagonists: a survey of computational studies ME Sobhia, R Singh, P Kare, S Chavan Expert opinion on drug discovery 5 (6), 543-557	2010
51	Probing interaction requirements in PTP1B inhibitors: a comparative molecular dynamics study R Kumar, RN Shinde, D Ajay, ME Sobhia Journal of chemical information and modeling 50 (6), 1147-1158	2010
52	RATIONAL DESIGN OF PEPTIDES DERIVED FROM AUTOINHIBITORY REGION: AN IN SILICO APPROACH FOR PKC beta II INHIBITION BK Grewal, P Divya, K Jain, D Ajay, ME Sobhia MEDICINAL CHEMISTRY RESEARCH 19, S58-S59	2010
53	FIRST IN SILICO STUDY OF HUMAN LEUKOCYTE ANTIGEN-RELATED PHOSPHATASE: PHARMACOPHORE, VIRTUAL SCREENING AND DOCKING BK Grewal, D Ajay, K Jain, ME Sobhia MEDICINAL CHEMISTRY RESEARCH 19, S62-S62	2010
54	ROLE OF alpha 7 HELIX IN THE BINDING OF PTP-1B ALLOSTERIC INHIBITORS R Shinde, ME Sobhia MEDICINAL CHEMISTRY RESEARCH 19, S121-S122	2010
55	Fingerprint directed scaffold hopping for identification of CCR2 antagonists PC Nair, ME Sobhia Journal of chemical information and modeling 48 (9), 1891-1902	2008
56	Comparative QSTR studies for predicting mutagenicity of nitro compounds PC Nair, ME Sobhia Journal of Molecular Graphics and Modelling 26 (6), 916-934	2008
57	Quantitative structure activity relationship studies on thiourea analogues as influenza virus neuraminidase inhibitors PC Nair, ME Sobhia European journal of medicinal chemistry 43 (2), 293-299	2008
58	Probing the structural and topological requirements for CCR2 antagonism: holographic QSAR for indolopiperidine derivatives K Srikanth, PC Nair, ME Sobhia Bioorganic & medicinal chemistry letters 18 (4), 1450-1456	2008
59	Quantitative structure activity relationship studies on thiourea analogues as influenza virus neuraminidase inhibitors	2008

	PC Nair, ME Sobhia European journal of medicinal chemistry 43 (2), 293-299	
60	Probing the structural and topological requirements for CCR2 antagonism: holographic QSAR for indolopiperidine derivatives K Srikanth, PC Nair, ME Sobhia Bioorganic & medicinal chemistry letters 18 (4), 1450-1456	2008
61	QSAR studies on CCR2 antagonists with chiral sensitive hologram descriptors PC Nair, K Srikanth, ME Sobhia Bioorganic & medicinal chemistry letters 18 (4), 1323-1330	2008
62	Characterization of solid-state forms of mebendazole S Kumar, G Chawla, ME Sobhia, AK Bansal Die Pharmazie-An International Journal of Pharmaceutical Sciences 63 (2 ...	2008
63	CoMFA based de novo design of pyridazine analogs as PTP1B inhibitors PC Nair, ME Sobhia Journal of Molecular Graphics and Modelling 26 (1), 117-123	2007
64	Design of Allosteric Ligands Using Computer Aided DrugDesign(CADD) Techniques. Khurana J, Nair PC and Sobhia ME; CRIPS 2006	2006
65	l-Menthol as new scaffold for designing chiral phase-transfer catalysts S Kumar, ME Sobhia, U Ramachandran Tetrahedron: Asymmetry 16 (15), 2599-2605	2005
66	Additivity of molecular fields: CoMFA study on dual activators of PPARα and PPARγ S Khanna, ME Sobhia, PV Bharatam Journal of medicinal chemistry 48 (8), 3015-3025	2005
67	Comparative molecular similarity indices analysis (CoMSIA) studies of 1, 2-naphthoquinone derivatives as PTP1B inhibitors ME Sobhia, PV Bharatam Bioorganic & medicinal chemistry 13 (6), 2331-2338	2005
68	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) R Thilagavathi, R Kumar, V Aparna, ME Sobhia, B Gopalakrishnan, ... Bioorganic & medicinal chemistry letters 15 (4), 1027-1032	2005
69	3D-QSAR studies of pyruvate dehydrogenase kinase inhibitors	2004

	based on a divide and conquer strategy TL Aboye, ME Sobhia, PV Bharatam Bioorganic & medicinal chemistry 12 (10), 2709-2715	
70	3D-QSAR CoMFA CoMSIA studies on indomethacin derivatives as selective cyclooxygenase-2 inhibitors M AROCKIA BABU, ME Sobhia, M Sharma, S Khanna, PV Bharatam, ... Indian journal of pharmaceutical sciences 66 (5), 613-620	2004
71	3D-QSAR studies of indole derivatives as phosphodiesterase IV inhibitors AK Chakraborti, B Gopalakrishnan, ME Sobhia, A Malde European journal of medicinal chemistry 38 (11), 975-982	2003
72	Comparative molecular field analysis (CoMFA) of phthalazine derivatives as phosphodiesterase IV inhibitors AK Chakraborti, B Gopalakrishnan, ME Sobhia, A Malde Bioorganic & medicinal chemistry letters 13 (15), 2473-2479	2003
73	3D-QSAR studies on thieno [3, 2-d] pyrimidines as phosphodiesterase IV inhibitors AK Chakraborti, B Gopalakrishnan, ME Sobhia, A Malde Bioorganic & medicinal chemistry letters 13 (8), 1403-1408	2003
74	3D-QSAR Analysis of Substituted 1, 3, 4-triaryl-3-pyrrolin-2-ones as Selective Cyclooxygenase-2-Inhibitors AK Chakraborti, B Gopalakrishnan, ME Sobhia, A Malde Indian J. Pharm. Sci 65 (3), 244-249	2003
75	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 GR Desiraju, B Gopalakrishnan, RKR Jetti, A Nagaraju, D Raveendra, ... Journal of medicinal chemistry 45 (22), 4847-4857	2002
76	Computer-aided design of selective COX-2 inhibitors: comparative molecular field analysis and docking studies of some 3, 4-diaryloxazolone derivatives GR Desiraju, J Sarma, D Raveendra, B Gopalakrishnan, R Thilagavathi, ... Journal of Physical Organic Chemistry 14 (7), 481-487	2001
77	RESEARCH ARTICLES-Computer-aided design of selective COX-2 inhibitors: Comparative molecular field analysis and docking studies of some 3, 4-diaryloxazolone derivatives GR Desiraju, J Sarma, D Raveendra, B Gopalakrishnan, R Thilagavathi, ... Journal of Physical Organic Chemistry 14 (7), 481-487	2001

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