



Professor

Molecular Modeling Lab (MML)

Department of Pharmaceutical Sciences & Drug Research

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Dr. OM SILAKARI (M. Pharm.; PhD)

PERSONAL DETAILS Dr. Silakari was born on 27-11-1973 in Indore, Madhya Pradesh. He is married to Mrs. Bhawna Vyas, and also has two kids' Prajwal and Aadhya.

EDUCATION M. PHARMACY

In Pharmaceutical Chemistry

“QSAR Analysis of Selective COX-2 Inhibitors Using Computerized Molecular Modeling Techniques”.

Ph. D.

In Pharmaceutical Sciences

“Molecular Modeling of Some NSAIDS: Synthesis and Biological Agents”.

RESEARCH INTERESTS AREA OF SPECIALIZATION

Pharmaceutical Chemistry

AREA OF RESEARCH

Computer Assisted Drug Design (CADD), QSAR, and chemical synthesis.

SPECIFIC RESEARCH TOPICS

Computer assisted designing of anti-inflammatory agents for various targets like mPGES-1, SYK, ITK, IRAK-4, TACE, P2X₇, PKC- θ , JAKs, cFMS, ZAP-70 etc.

Computational studies on various kinases such as PI3K α , ITK, EGFR, ALK, cMET, FGFR, ErbB2 and IRAK-4.

Synthesis of benzimidazole, flavones, acridone, oxindole, thiazolidinedione, and iminopyrimidines molecules for various activities.

Computational analysis and designing of inhibitor molecules for anti-cancer targets, e.g. PI3K α , and farnesyl transferase.

**RESEARCH AND
TEACHING EXPERIENCE**

FOR TEACHING

2020-till date

Professor, Department of Pharmaceutical Sciences & Drug Research, Punjabi University, Patiala.

2017-2020

Associate Professor, Department of Pharmaceutical Sciences & Drug Research, Punjabi University, Patiala.

2009 to 2017

Assistant Professor, Department of Pharmaceutical Sciences & Drug Research, Punjabi University, Patiala.

2005 to 2009

Lecturer, Department of Pharmaceutical Sciences & Drug Research, Punjabi University, Patiala.

2003-2004

School of Pharmacy, Devi Ahilya Vishwavidyalaya, Indore, MP (India).

2000-2003

Department of Pharmaceutical Sciences, Dr. H.S. Gour University Sagar, MP (India).

FOR RESEARCH

2001-2004

CSIR Senior Research Fellow (SRF) at Department of Pharmaceutical Sciences, Dr. H. S. Gour University, Sagar, MP.

1997-1999

UGC Junior Research Fellow (JRF) at Department of Pharmaceutical Sciences, Dr. H. S. Gour University, Sagar, MP.

**TEACHING
RESPONSIBILITIES**

UNDER GRADUATE LEVEL

Organic Chemistry, Inorganic Chemistry, Medicinal Chemistry, and Biochemistry.

POST GRADUATE LEVEL

Computer Aided Drug Design, Principles of Drug Discovery, Chemistry of Natural Products, Advanced Medicinal Chemistry

Ph.D. LEVEL

Spectral Analysis (for PhD course work students).

**PROFESSIONAL
RESPONSIBILITIES**

Member of Departmental Research Board, Department of Pharmaceutical Sciences and Drug Research, PUP.

Member of Academic Council of Department of Pharmaceutical Sciences and Drug Research, PUP.

Member of Board of Study of Faculty of Medicine, PUP.
Member of Board of Studies in Department of Pharmaceutical Sciences and Drug Research, PUP.
Member of the Admission Committee of the Department of Pharmaceutical Sciences and Drug Research, PUP.
In-charge of Anti-ragging committee of Department of Pharmaceutical Sciences and Drug Research, PUP.
Co-coordinator of '*Pharmafest*', Department of Pharmaceutical Sciences and Drug Research, PUP (2010-2012).

**MEMBERSHIPS OF
SCIENTIFIC
COMMUNITIES**

Life member of Punjab Academy of Sciences (Membership No. 1087).
Registered Pharmacist of M.P. Pharmacy Council.
Member of Environmental Society of Punjabi University.
Life member of IPA (Indian Pharmaceutical Association)
Life member of APTI (Association of Pharmaceutical Teachers of India)

**REFRESHER/ORIENTATI
ON**

Refresher courses of 21 days at Academic Staff College, Punjabi University, Patiala.
Orientation course of 27 days Academic Staff College, Punjabi University, Patiala.
UGC Sponsored Short Term Course of 7 days at UGC-Human Resource Development Centre, Punjabi University, Patiala.

**PROJECTS AWARDED
WITH FUNDING**

A Major Research Project of INR 12 lacs (approx.) from UGC on topic "Computer Based Molecular Modeling for Designing of Multi-targeted Agents for Various Inflammatory Disorders: Synthesis and Biological Evaluation". (Completed)
A Major Research Project of INR 15 lacs from CSIR on topic "In-silico Designing of Multi-Targeted Agents for the Treatment of Diabetic Complications". (Completed).
A Major Research Project of INR 20 lacs (approx.) from DBT on topic "Designing of Novel Kinase Inhibitors for Treatment of Lung Cancer". (Completed).
A major Research Project of INR 58 Lacs (approx.) from ICMR entitled "Bioinformatics Based analysis of tumoral drug inactivating enzymes to manage the pharmacokinetic resistance". (Completed).
Bioinformatics centre awarded by Department of Biotechnology (DBT) of INR 75 Lacs (approx.) entitled "Centre on Drug Design, Disposition and Toxicoinformatics" (Ongoing).
A Major Research Project of INR 18 Lacs (approx.) from ICMR entitled "Computer Assisted Optimization of Polymer-Mucin Interaction for Nose to Brain Delivery of Anti-Alzheimer's Drug" (Ongoing)
A Major Research Project of INR 18 Lacs from DST entitled "Deciphering molecular

signature for resistance to some kinase inhibitors used in the treatment of non-small cell lung cancer (NSCLC): A bioinformatics approach" (Recently approved)
Seven students received SRF from various funding agencies like ICMR, DST etc.

FELLOWSHIPS AWARDED UGC Junior Research Fellow (JRF) at Department of Pharmaceutical Sciences, Dr. H. S. Gour University, Sagar, MP (1997-1999).

CSIR Senior Research Fellow (SRF) at Department of Pharmaceutical Sciences, Dr. H. S. Gour University, Sagar, MP (2000-2004).

**INVITED
LECTURES
DELIVERED**

Delivered an invited talk on topic "Computerized Molecular Modeling" at National Conference organized by Adesh Institute of Pharmacy and Biomedical Sciences, Bathinda (Punjab).

Delivered an invited talk on topic "Computer Aided Molecular Modeling" at National Conference organized by Hans Raj Maha Vidyalaya, Jalandhar (Punjab).

Delivered an invited talk on topic "Computer Aided Molecular Modeling: Rational Tool for Drug Designing & Discovery" at National Conference organized by Hans Raj Maha Vidyalaya, Jalandhar (Punjab).

Delivered an invited talk on topic "Pharmacophore Mapping: A Tool for Rational Drug Design" at Computer aided Drug Design: Hands-on Workshop organized by University Institute of Pharmaceutical Sciences, Panjab University, Chandigarh (Punjab).

Delivered an invited talk on topic "Computer Aided Drug Design" at National Conference organized by Rayat-Bahra Institute of Pharmacy, Hoshiarpur (Punjab).

Delivered an invited talk on topic "Pharmacophore Mapping: A Tool for Rational Drug Design" at National level Workshop on Drug Design & Discovery organized by Institute of Life Sciences, Bhubaneshwar, Orissa (2016).

Delivered an invited talk on topic "Pharmacophore Mapping: A Tool for Rational Drug Design" at National level Workshop on Drug Design & Discovery organized by Institute of Life Sciences, Bhubaneshwar, Orissa (2017).

RESEARCH STUDENTS GUIDED

AT Ph.D. LEVEL

Sr. No	Course	Name of Candidate	Registered	Awarded
1	Ph.D.	Rajesh Kumar	21/09/2009	28/05/2015
2	Ph.D.	Yogita Bansal	22/09/2009	28/05/2015
3	Ph.D.	Malkeet Singh Bahia	16/02/2010	19/11/2014
4	Ph.D.	Gaganpreet Kaur	05/03/2012	2019
5	Ph.D.	Maninder Kaur	07/10/2013	26/05/2017
6	Ph.D.	Manjinder Singh	07/10/2013	23/04/2018
7	Ph.D.	Navriti	15/09/2015	23/08/2018
8	Ph.D.	Pankaj Kumar Singh	11/08/2016	15/05/2019
9	Ph.D.	Shalki	25/07/2017	18/02/2022
10	Ph.D.	Himanshu Verma	24/05/2018	-
11	Ph.D.	Manoj Kumar	09/11/2020	-
12	Ph.D.	Baddipadige Raju	09/11/2020	-
13	Ph.D.	Gera Narendra	09/11/2020	-
14	Ph.D.	Mohit Motiwale	09/11/2022	-

AT POST GRADUATE LEVEL

Sr. No	Course	Name of Candidate	Degree Awarded
1	M. Pharm	Tabish Equbal	2007
2	M. Pharm	Neha Kansal	2008
3	M. Pharm	Tarnvir Sammi	2008
4	M. Pharm	Navneet Kaur	2008
5	M. Pharm	Malkeet Singh	2009
6	M. Pharm	Neha Bagga	2009
7	M. Pharm	Vijay Singh Ghorela	2010
8	M. Pharm	Vikas Bagga	2010
9	M. Pharm	Sukhvir Chand	2011
10	M. Pharm	Nisha Mehta	2011
11	M. Pharm	Maninder Kaur	2012
12	M. Pharm	Archna Kumari	2012
13	M. Pharm	Haneesh Jasuja	2013
14	M. Pharm	Navriti Chadha	2013
15	M. Pharm	Pratibha Duggal	2014
16	M. Pharm	Siddharth Upadhyay	2014
17	M. Pharm	Akashdeep Singh	2015
18	M. Pharm	Nalini	2015
19	M. Pharm	Disha Pathak	2016
20	M. Pharm	Himanshu Verma	2017
21	M. Pharm	Aanchal Kashyap	2017
22	M. Pharm	Swati Kapil	2018
23	M. Pharm	Vivek Panwar	2018
24	M. Pharm	Manoj Kumar	2019
25	M. Pharm	Mohit	2019
26	M. Pharm	Kajal Sharma	2020
27	M. Pharm	Kanupriya Mahajan	2020
28	M. Pharm	Manmeet Singh	2021
29	M. Pharm	Priyanka Bhandu	2021
30	M. Pharm	Bhavna Sharma	2022
31	M. Pharm	Himani	2022

CONFERENCES
ATTENDED AND
POSTER/ORAL
PRESENTATIONS

XVIII M.P. Young Scientist Congress (2003).

UGC Sponsored National Seminar on Drug Delivery and Pharmacovigilance (2012).

National Seminar on Health, Fitness and Sports Technology (2012).

National Seminar on Genetically Modified Foods: Current Scenario (2012).

National Symposium on Current Trends in Liposome Research (1998).

National Science Day Seminar on Role of Science in Sustainable Development (2000).

IPRs Awareness Workshop (2008).

XIX M.P. Young Scientist Congress (2004).

Malkeet Singh Bahia, Sukhvir Chand and **Om Silakari** (2011) "Designing of New Selective TACE Inhibitors Using Combined Computerized Molecular Modeling Techniques", paper presented at '14th Punjab Science Congress' organized by SLIET, Longowal, Sangrur (Punjab).

Maninder Kaur, Sukhvir Chand, Archana Kumari, Malkeet Singh Bahia and **Om Silakari** (2011) "Receptor Guided Atom Based 3D QSAR Analysis of Thieno[2,3-b]pyridine-5-carbonitrile Inhibitors of PKC- θ ", paper presented at 'APTI 16th Annual National Convention on Reframing Pharmacy Education Through Need Based Approach' organized by ISF College of Pharmacy, Moga (Punjab).

Archana Kumari, Nisha Mehta, Maninder Kaur, Malkeet Singh Bahia and **Om Silakari** (2011) "CoMFA and CoMSIA Analyses of Triazole Derivatives for its P2X₇ Antagonism", paper presented at 'APTI 16th Annual National Convention on Reframing Pharmacy Education through Need Based Approach' organized by ISF College of Pharmacy, Moga (Punjab).

Malkeet Singh, Archana Kumari, Maninder Kaur and **Om Silakari** (2011) "A Combination of QM, Pharmacophore Modelling and QSAR Analyses to Explore the Biological Potential of Urea Derivatives as mPGES-1 Inhibitors", paper presented at 'APTI 16th Annual National Convention on Reframing Pharmacy Education Through Need Based Approach' organized by ISF College of Pharmacy, Moga (Punjab).

Malkeet Singh Bahia and **Om Silakari** (2011) "Exploring the Essential

Structural Feature Requirement for Biological Potential of Cyclopropyl Derivatives of TACE Inhibitors”, paper presented at ‘National Seminar on Current Scenario in Pharmaceutical Sciences’ organized by Adesh Institute of Pharmacy and Biomedical Sciences, Bathinda (Punjab). **(AWARDED AS BEST POSTER)**

Malkeet Singh Bahia (2011) Attended a DBT & UGC Sponsored National Seminar on ‘BIOTECH VISTAS-2011’ organized by Department of Biotechnology, Punjabi University, Patiala (Punjab).

Nisha Mehta, Sukhvir Chand, Malkeet Singh Bahia and **Om Silakari** (2011) “3D QSAR Study to Explore Essential Structural Features Requirement of 4,5-Diaryl Imidazolines as Novel P2X₇ Receptor Antagonists”, presented a paper at ‘3rd National Conference on Recent Advances in Chemical and Environmental Sciences’ organized by M.M. Modi College, Patiala (Punjab). **(BEST POSTER).**

Sukhvir Chand, Nisha Mehta, Malkeet Singh Bahia and **Om Silakari** (2011) “3D-QSAR Study Using Docking Based Molecular Alignment for the Structural Requirement of Amino Pyrimidines as PKC- θ Inhibitors”, presented a paper at ‘3rd National Conference on Recent Advances in Chemical and Environmental Sciences’ organized by M.M. Modi College, Patiala (Punjab).

Sukhvir Chand, Nisha Mehta, Malkeet Singh Bahia and **Om Silakari** (2011) “PKC- θ : A New Promising Target Towards the Treatment of Inflammatory Disorders”, presented a paper at ‘14th Punjab Science Congress’ organized by SantLongowal Institute of Engineering and Technology, Longowal, Sangrur (Punjab).

Malkeet Singh Bahia and **Om Silakari** (2009) “Three Dimensional Pharmacophore Modeling of γ -Secretase Inhibitors Using Catalyst HypoGen Program”, oral presentation at ‘National conference on Innovations in Drug Discovery and Research (IDDR)’ organized by Punjabi University, Patiala in March 2009.

Maninder Kaur, Archana Kumari, Malkeet Singh Bahia and **Om Silakari** (2012) “Exploring the Importance of Water Molecules for Docking and Receptor Guided 3D QSAR Analysis of Naphthyridine Derivatives as Syk Inhibitors” presented a paper at ‘15th Punjab Science Congress’ organized by Guru Nanak Dev University, Amritsar (Punjab).

Malkeet Singh Bahia and **Om Silakari** (2012) “Combined Molecular Modeling Strategy for Designing of New Selective TACE Inhibitors” oral presentation delivered at ‘15th Punjab Science Congress’ organized by Guru Nanak Dev

University, Amritsar (Punjab). **(PUNJAB YOUNG SCIENTIST AWARD 2012).**

Archana Kumari, Maninder Kaur and **Om Silakari** (2012) "3D-QSAR Analysis of Anilinoquinoline Inhibitors of cFMS Kinase Utilizing Field Based Alignment" presented a paper at '15th Punjab Science Congress' organized by Guru Nanak Dev University, Amritsar (Punjab).

Maninder Kaur, Malkeet Singh Bahia and **Om Silakari** (2012) "Development of Three Dimensional Model for Human Melacortin-4 Receptor Antagonists Using Ligand Based Molecular Modeling Technique" presented a paper at 'National Conference on Recent Advances in Chemical and Environmental Sciences' organized by M.M. Modi College, Patiala (Punjab).

Malkeet Singh Bahia, Sukhvir Chand and **Om Silakari** (2011) "PKC- θ : A New Promising Target towards the Treatment of Inflammatory Disorders", paper presented at '14th Punjab Science Congress' organized by SLIET Longowal, Sangrur (Punjab).

Haneesh Jasuja and **Om Silakari** (2013) "Computer Assisted Designing of Multi-target Inhibitors of Janus Kinase-3 (JAK-3) and Spleen Tyrosine Kinase (SYK) Enzymes" oral presentation delivered at '15th Punjab Science Congress' organized by Baba Farid University of Health Sciences, Faridkot (Punjab). Navriti

Chadha and **Om Silakari** (2013) "Identification of PI3K α Inhibitors:

3D-QSAR Based Designing Using Implementation of Hybrid Monte-Carlo Algorithm" oral presentation delivered at '15th Punjab Science Congress' organized by Baba Farid University of Health Sciences, Faridkot (Punjab).

Maninder Kaur and **Om Silakari** (2013) "Designing of New Dual Inhibitors of cFMS and JAK-3 Using Multiple Molecular Modeling Approaches", oral presentation delivered at '15th Punjab Science Congress' organized by Baba Farid University of Health Sciences, Faridkot (Punjab).

Malkeet Singh Bahia and **Om Silakari** (2012) "Consideration of Receptor Flexibility and Water Importance for Receptor Guided 3D-QSAR Analysis of Benzimidazole Derivatives as Interleukin-2 Inducible T-cell kinase (ITK) Inhibitors", paper presented at 'International Conference on Industrial Biotechnology' organized by Department of Biotechnology, Punjabi University, Patiala (Punjab).

Haneesh Jasuja, Sukhvir Chand and **Om Silakari** (2012) "Receptor Guided 3D-QSAR Analysis of Thieno[2,3-b]pyridine-5-carbonitrile Inhibitors of Protein Kinase C theta (PKC- θ)", paper presented at 'International Conference on Industrial Biotechnology' organized by Department of Biotechnology, Punjabi

University, Patiala (Punjab).

Navriti Chadha and **Om Silakari** (2012) "Implementation of Hybrid Monte Carlo Method to Refine Receptor-ligand Conformations for 3D-QSAR Analysis of Imidazo[1,2-a]pyrazine Inhibitors of Phosphoinositide 3-kinase Alpha (PI3K α)", paper presented at 'International Conference on Industrial Biotechnology' organized by Department of Biotechnology, Punjabi University, Patiala (Punjab).

Maninder Kaur, Malkeet Singh Bahia and **Om Silakari** (2012) "Uncovering the Essential Structural Features of Phenanthrene mPGES-1 Enzyme Inhibitors Using 3D-QSAR Analysis", paper presented at 'International Conference on Industrial Biotechnology' organized by Department of Biotechnology, Punjabi University, Patiala (Punjab).

Haneesh Jasuja and **Om Silakari** (2013) "Computer Aided Designing of Dual Inhibitors of JAK-1 and 3 Enzymes", poster presented at '2nd International Conference on Emerging Trends in Drug Research and Development' organized by Dhanvantary Pharmacy College, Kim, Surat (Gujarat).

Navriti Chadha and **Om Silakari** (2013) "3D Pharmacophore Mapping of PI3K α Inhibitors", poster presented at 'Indian Science Congress Association' organized by Punjabi University, Patiala (Punjab).

Haneesh Jasuja and **Om Silakari** (2012) "Determination of Relative Importance of Amino Acid Residues for JAK-1 Inhibition Using Docking Analysis" poster presented at 'Indian Pharmacy Graduates Association National Convention' organized by Kurukshetra University, Kurukshetra (Haryana) **(BEST POSTER)**

Malkeet Singh Bahia and **Om Silakari** (2013) "Exploring the Essential Structural Features of Benzimidazole Derivatives Required for Dual Inhibitory Activity against ITK and IRAK-4 Kinases Using 3D-QSAR Methodology" poster presented at '3rd Indo German Conference on Modeling, Chemical and Biochemical (Re)activity' organized by NIPER, Mohali (Punjab).

Maninder Kaur, Archana Kumari, Malkeet Singh Bahia and **Om Silakari** (2013) "Molecular Docking and Pharmacophore Mapping based Designing of novel Spleen Tyrosine Kinase Inhibitors" poster presented at '3rd Indo German Conference on Modeling, Chemical and Biochemical (Re)activity' organized by NIPER, Mohali (Punjab).

Manjinder Singh and **Om Silakari** (2015) An oral presentation in National Conference on the topic Advancements, Opportunities and Future Vision of

Indian Scenario of Pharmaceutical Education and Research, 3-4 April 2015 organized by Rayat-Bahra Institute of Pharmacy, Hoshiarpur. **(1st Position)**

Manjinder Singh and **Om Silakari** (2015) An oral presentation in International Conference (INNOPHARM1) on the topic 'Novel Frontiers in Pharmaceutical and Health Sciences, 10-11 Oct, 2015' organized by M.P. Council of Science and Technology, Bhopal, M.P. India **(3rd Position)**

Maninder Kaur and **Om Silakari** (2015) A poster presented on the topic 'Designing and synthesis of Novel Zeta-Chain associated Protein Tyrosine Kinase 70kDa (ZAP-70) Inhibitors by Molecular Docking and Pharmacophore Mapping based Scaffold Hopping' in International Conference on the topic Molecular Pharmacology, Drug Discovery and Nanopharmaceuticals (MPDDNP), 27th-28th March, 2015 organized by Chitkara University, Rajpura, Punjab. **(2nd Position)**

Maninder Kaur and **Om Silakari** (2015). A poster presented on the topic 'Hierarchical virtual screening based designing of dual inhibitors of colony-stimulating factor-1 receptor (cFMS) and Janus kinase-3 (JAK3)' in National Conference on the topic Advancements, Opportunities and Future Vision of Indian Scenario of Pharmaceutical Education and Research, 3-4 April 2015 organized by Rayat-Bahra Institute of Pharmacy, Hoshiarpur. **(1st position)**

Manjinder Singh and **Om Silakari** (2016) A poster presentation award at UGC-UKIERI international seminar on "Nanotherapeutics & Crystal Engineering: Challenges and Future Perspectives" 08th, February 2016, organized by DPSDR, Punjabi University, Patiala & Centre for Pharmaceutical Engineering Science, University of Bradford, United Kingdom at DPSDR, Punjabi University, Patiala. **(1st Position)**

Manjinder Singh and **Om Silakari** (2016) A poster presentation at 5th Annual International Conference & Exhibition on Imparting innovative knowledge and translational & research towards public health care" 4-5th March, 2016 organized by Society of Pharmaceutical Education & Research (SPER) at Chandigarh College of Pharmacy, Landran, Chandigarh, India. **(1st Position)**

Manjinder Singh and **Om Silakari** (2016) A poster presentation at 2nd Annual National Convention of APTI (Punjab State Branch) on 'Emerging Scenario in Human Resource Development for Pharmacy Profession' 18th-19th March, 2016 organized by APTI at Government Polytechnic College for girls, Patiala. **(1st Position)**

Maninder Kaur and **Om Silakari** (2015). A poster presentation in 6th

International Conference on 'Bioinformatics and System Biology' on the topic 'Bridging Bioinformatics and System Biology: A peek into Future, 22-23 August, 2016, organized by OMICS at **Philadelphia, USA**.

Himanshu Verma and **Om Silakari** (2017) A poster presentation in International Conference on Drug Design, 7-9 April, 2017, organized by Schrodinger at Jawaharlal Nehru University, New Delhi. (**3rd Position**)

Pankaj Kumar Singh and **Om Silakari** (2017) A poster presentation in International Conference on Drug Design, 7-9 April, 2017, organized by Schrodinger at Jawaharlal Nehru University, New Delhi.

Om Silakari (2017) as a poster evaluator in International Conference on Drug Design, 7-9 April, 2017, organized by Schrodinger at Jawaharlal Nehru University, New Delhi.

Om Silakari (2017) as a Resource Person (oral presentation session) in 3rd Annual Convention of APTI Punjab (APTICON Punjab) held at University School of Pharmaceutical Sciences, Rayat-Bahra University, Mohali on April 13-14, 2017,

REVIEWER OF JOURNALS

Chemical Biology and Drug Design (Wiley)
Journal of Molecular Graphics and Modeling (Elsevier)
European Journal of Medicinal Chemistry (Elsevier)
Medicinal Chemistry Research (Springer)
SAR and QSAR in Environmental Research (Taylor and Francis)
Letters in Drug Design & Discovery (Bentham)
Medicinal Chemistry (Bentham)
Arabian Journal of Chemistry (Elsevier)
Bioorganic and Medicinal Chemistry (Elsevier)
Journal of Saudi Chemical Society (Elsevier)
Bioorganic and Medicinal Chemistry Letters (Elsevier)

RESEARCH PROFILE

Total Citations 5761
h-index 33
i10-index 87

PAPER PUBLICATIONS

Sr. No.	Author(s)	Title	Name of Journal	Year
1	Singh, M., Verma, H., Gera, N., Baddipadige, R., Choudhary, S., Bhandu, P., & Silakari, O.	Evaluation of Cordyceps militaris steroids as anti-inflammatory agents to combat the Covid-19 cytokine storm: a bioinformatics and structure-based drug designing approach	Journal of Biomolecular Structure and Dynamics	

2	Raju, B., Verma, N., Narendra, G., Silakari, O., & Sapra, B.	Classification of Potent and Weak Penetration Enhancers Using Multiple Feature Selection Methods and Machine Learning Models	Journal of Pharmaceutical Innovation	2023
3	Narendra, G., Raju, B., Verma, H., Kumar, M., Jain, S. K., Tung, G. K., ... & Silakari, O.	Raloxifene and bazedoxifene as selective ALDH1A1 inhibitors to ameliorate cyclophosphamide resistance: A drug repurposing approach	International Journal of Biological Macromolecules	2023
4	Bhandu, P., Verma, H., Raju, B., Narendra, G., Choudhary, S., Singh, M., ... & Silakari, O.	Identification of natural peptides from "PlantPepDB" database as anti-SARS-CoV-2 agents: A protein-protein docking approach	Phytomedicine Plus	2023
5	Sharma, H., Raju, B., Narendra, G., Kumar, M., Verma, H., Sharma, B., ... & Silakari, O.	In silico guided designing of optimized benzochalcones derivatives as potent CYP1B1 inhibitors: An integrated in vitro and ONIOM study	Journal of Molecular Graphics and Modelling	2023
6	Singh, M., Verma, H., Bhandu, P., Kumar, M., Narendra, G., Choudhary, S., ... & Silakari, O.	Network Analysis Guided Designing of Multi-Targeted Anti-Fungal Agents: Synthesis and Biological Evaluation	Journal of Molecular Structure	2023
7	Sharma, H., Raju, B., Narendra, G., Motiwale, M., Sharma, B., Verma, H., & Silakari, O.	QM/MM Studies on Enzyme Catalysis and Insight into Designing of New Inhibitors by ONIOM Approach: Recent Update	Chemistry Select	2023
8	Verma, H., Doshi, J., Narendra, G., Raju, B., Singh, P. K., & Silakari, O. (2023).	Energy decomposition and waterswapping analysis to investigate the SNP associated DPD mediated 5-FU resistance	SAR and QSAR in Environmental Research	2023
9	Bhandu, P., Verma, H., Singh, M., Kumar, M., Narendra, G., Choudhary, S., ... & Silakari, O.	Rational designing of quinazolin-4 (3H)-one based ALR2 inhibitors: Synthesis and biological evaluation	Journal of Molecular Structure	2023
10	Kumar, M., Singh, P. K., Choudhary, S., & Silakari, O.	Hydantoin based dual inhibitors of ALR2 and PARP-1: Design, synthesis, in-vitro and in-vivo evaluation	Bioorganic Chemistry	2022
11	Raju, B., Sapra, B., & Silakari, O.	3D-QSAR assisted identification of selective CYP1B1 inhibitors: an effective bioisosteric replacement/molecular docking/electrostatic complementarity analysis	Molecular Diversity	2022
12	Raju, B., Verma, H., Narendra, G., Sapra, B., & Silakari, O.	Multiple machine learning, molecular docking, and ADMET screening approach for identification of selective inhibitors of CYP1B1	Journal of Biomolecular Structure and Dynamics	2022

13	Narendra, G., Choudhary, S., Raju, B., Verma, H., & Silakari, O.	Role of genetic polymorphisms in drug-metabolizing enzyme-mediated toxicity and pharmacokinetic resistance to anti-cancer agents: a review on the pharmacogenomics aspect	Clinical Pharmacokinetics	2022
14	Verma, H., Narendra, G., Raju, B., Singh, P. K., & Silakari, O.	Dihydropyrimidine Dehydrogenase-Mediated Resistance to 5-Fluorouracil: Mechanistic Investigation and Solution	ACS Pharmacology & Translational Science	2022
15	Verma, H., Narendra, G., Raju, B., Kumar, M., Jain, S. K., Tung, G. K., ... & Silakari, O.	3D-QSAR and scaffold hopping based designing of benzo [d] oxazol-2 (3H)-one and 2-oxazolo [4, 5-b] pyridin-2 (3H)-one derivatives as selective aldehyde dehydrogenase 1A1 inhibitors: synthesis and biological evaluation	Archiv der Pharmazie	2022
16	Raju, B., Narendra, G., Verma, H., Kumar, M., Sapra, B., Kaur, G., ... & Silakari, O.	Machine learning enabled structure-based drug repurposing approach to identify potential CYP1B1 inhibitors	ACS omega	2022
17	Mudi, P. K., Mahato, R. K., Verma, H., Panda, S. J., Purohit, C. S., Silakari, O., & Biswas, B.	In silico anti-SARS-CoV-2 activities of five-membered heterocycle-substituted benzimidazoles.	Journal of molecular structure	2022
18	P Sharma, B Raju, G Narendra, B Sapra, O Silakari	Molecular Docking, Dynamics, and WaterSwap Analysis to Identify Anti-aggregating Agents of Insulin and IFN- β .	Applied Biochemistry and Biotechnology	2022
19	K Sharma, S Choudhary, O Silakari	Portraying molecular modulation and therapeutic aspects of psoriasis: Retrospection and current status	Journal of Molecular Structure	2021
20	N Gautam, H Verma, S Choudhary, S Kaur, O Silakari	Functional relationship of SNP (Ala490Thr) of an epigenetic gene EZH2 results in the progression and poor survival of ER+/tamoxifen treated breast cancer patients.	Journal of genetics	2021
21	G Narendra, B Raju, H Verma, O Silakari	Identification of potential genes associated with ALDH1A1 overexpression and cyclophosphamide resistance in chronic myelogenous leukemia using network analysis.	Medical Oncology	2021
22	Narendra G, Raju B, Verma H, Sapra B, Silakari O.	Multiple Machine Learning Models Combined with Virtual Screening and Molecular Docking to Identify	Journal of Molecular Graphics and Modelling	2021

23	Sharma K, Choudhary S, Silakari O.	Selective Human ALDH1A1 inhibitors. Portraying molecular modulation and therapeutic aspects of psoriasis: Retrospection and current status.	Journal of Molecular Structure	2021
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Conflict of Interest

I hereby declare that there is no conflict of interest (such as financial or personal interests) related to this proposal.

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Om Silakari