



Dr. Sanjeev Kumar Singh
Professor and Head i/c

Contact

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Academic Qualifications

Degree	Institution	Year	Branch	Class
D. Sc.	Alagappa University, Karaikudi, TN	2022	Bioinformatics	-
Ph. D.	CSJM University, Kanpur, UP	2004	Applied Chemistry	-
M. Sc.	Institute of Life Sciences, CSJM University, Kanpur, UP	2000	Life Sciences	First
B. Sc.	Christ Church College, CSJM University, Kanpur, UP	1998	Zoology, Botany, Chemistry	First

Teaching Experience		
Total Teaching Experience : 18 Years & 9 Months		
Position	Institution	Duration
Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	8 years 11 months (Continue)
Professor (On Lien)	Dept. of Data Science, Centre of Bio-Medical Research (CBMR), Sanjay Gandhi Post-Graduate Institute of Medical Sciences Campus, Lucknow, Uttar Pradesh - 226014	10 months
Associate Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	3 years
Reader	Dept. of Bioinformatics Alagappa University Karaikudi	3 years
Lecturer	CoE in Bioinformatics, School of Biotechnology, Madurai Kamaraj University	3 years

Research Experience		
Total Research Experience : 24 Year		
Position	Institution / University	Duration
Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	8 years 11 months (Continue)
Professor (On Lien)	Dept. of Data Science, Centre of Bio-Medical Research (CBMR), Sanjay Gandhi Post-Graduate Institute of Medical Sciences Campus, Lucknow, Uttar Pradesh - 226014	10 months
Associate Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	3 years
Reader	Dept. of Bioinformatics Alagappa University Karaikudi	3 years
Lecturer	CoE in Bioinformatics, School of Biotechnology, Madurai Kamaraj University	3 years
RA/Scientist-II	Pharmacoinformatics Division, NIPER, Mohali	1 year 9 months

Senior Research Fellow	Dept. of Chemistry, IET, CSJM University, Kanpur	1 year 6 months
Junior Research Fellow	Dept. of Chemistry, IET, CSJM University, Kanpur	2 years

Academic and Additional Responsibilities

S.No	Position	University Bodies	Period	
			From	To
1.	Head i/c	Dept. of Botany Alagappa University Karaikudi, Tamil Nadu	1 st Nov 2023	Continue
2.	Planning Board Member	Alagappa University, Karaikudi	2022	2025
3.	Coordinator for Rashtriya Uchchar Shiksha Abhiyan (RUSA 2.0)	Alagappa University, Karaikudi	Feb 2019	24th Nov 2022
4.	Nodal Officer for the “India International Science Festival (IISF) 2020	Alagappa University, Karaikudi	29 th Nov 2020	*
5.	Nodal Officer for Niti Aayog – Grant in Aid	Alagappa University, Karaikudi	25 th January 2019	*
6.	Special Officer (Projects)	Alagappa University, Karaikudi	2018	2019
7.	Special Officer (Funding Agencies)	Alagappa University, Karaikudi	July 2017	December 2017
8.	Coordinator of MHRD- Ek Bharat Shreshtha Bharat (EBSB)	Alagappa University, Karaikudi	2017	till date
9.	Deputy Coordinator, DST-FIST Program (Level-I)	Department of Bioinformatics, Alagappa University, Karaikudi	2017	*
10.	Department Coordinator of UGC-NAAC	Department of Bioinformatics, Alagappa University.	2017	2018
11.	Liaison Officer (to deal affairs between Alagappa University and other funding agencies such as UGC, DST, CSIR)	Alagappa University, Karaikudi	16 th Nov 2016	2019
11.	Special Invitee in Senate	Alagappa University, Karaikudi	2009	-

Areas of Research

Research Expertise: Structural bioinformatics and computer aided drug designing.

Research Fields:

- **Viroinformatics** : Advanced computation methods has been employed in identification of potential therapeutics against lethal viral targets such as **SARS-CoV2, HIV, HTLV, ZIKV and DENV**.
- **Cancer informatics** : Understanding the complex mechanism of cancer with the aid of *Insilico* studies on cancer targets such as Cyclin dependent Kinases (**CDKs**) and other causative agents like Human papilloma virus (**HPV**). These studies help in providing a better intuition to develop potent anti-cancer and anti-HPV compounds.
- **Bacteriology** : Elucidating the mechanistic insights of biofilm and spore forming bacterial species resulting in identification of potential anti-biofilm and anti-sporulation compounds, Other pathogens that have been targeted by my group are protozoan disease causing *Leishmaniasis*.
- **Lifestyle disorders**: We have also worked on human lifestyle disorders such as hypertension, diabetes and neurological disorder by targeting the Human G Protein Coupled Receptor (GPCR), pancreatic lipase and currently we are working in the autism disorder.

Research in my laboratory is extensively focused on these targets and designing various inhibitors to impede their functional importance on the premise of combined *in-silico* approaches including **Molecular Modelling, Biophysical methods, Structural Bioinformatics and Computational Biology**. My research team is working on understanding the relation between protein-protein/protein-Ligand complex structures and their function are carried out through the **Quantum Mechanical and Molecular Mechanical calculation (QM/MM calculation), MO/DFT prediction, Free energy calculation, Pharmacophore mapping and Quantum Polarized Ligand docking (QPLD)** as well as **induced Fit Docking**. In order to develop new models, Ab initio Quantum calculation, 3D-database searching & development, combinatorial library design, Optimization of lead compounds generated massive libraries of small molecules to screen against specific therapeutic processes. Additionally, my research group has developed the tool, converting the inhibition concentration (**IC50**) into **PIC50** which has recognized by the scientific society (<https://www.sanjeevslab.org/tools.html>).

Research Supervision / Guidance			
Program of Study		Completed	Ongoing
Research	PDF	04	1
	Ph.D	09	10
	M.Phil	09	-

Project	PG	52	6
	UG / Others	21	-

Publications				
International		National		Others
Journals	Conferences	Journals	Conferences	Books / Chapters / Monographs / Manuals
181	4	05	-	Edited Book: 1 Book Chapters: 40 Review articles: 11

Cumulative Impact Factor (as per JCR) : 661.27

h-index : 39

i10 index : 123

Total : 4783

Citations

Number of Thesis Evaluated/ Viva voce Examiner

Thesis Evaluated : 52

Viva voce Examiner : 32

Funded Research Projects					
Ongoing Projects: 5					
S.No	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
1.	DBT-NNP	2023	2025	Identification of Potential drug for Life Threatening disease (PI)	144.56
2.	DBT-BIC	2021	2025	Identification of Potential drug for Life Threatening disease (Co-PI)	183.88
3.	RUSA 2.0 - TBRP	2018	2024	Mechanistic insights to understand the virus-host interaction and the identification of next-generation drugs to combat viral infections (PI)	33.00

4.	Tamil Nadu – Higher Education Department	2020	2023	Scheme for Alternative Strategy to antibiotics in bacterial disease management at Alagappa University (PI)	100.00
5.	Tamil Nadu State Council for Higher Education (TANSCH), Chennai	2021	2024	Identification of the vital targets of dengue and Chikungunya, an expanding threat to public health in Tamil Nadu: A potential drug discovery approach (PI)	20.16

Completed Projects: 7

S.No	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
1.	MHRD, SPARC	2019	2022	Biophysics of Zika virus envelope protein, membrane fusion and inhibitor discovery	97.23
2.	DBT, New Delhi	2016	2019	In-Silico screening, theoretical calculation and in vitro studies for development of potential HIV1-PR inhibitors	19.51
3.	DBT-Twin Project with IIT, Guwahati	2014	2018	Identification of novel drug targets of Leishmania donovani: Studies on CAAX prenyl protease I and II of the pathogen.	73.69
4.	CSIR, New Delhi	2012	2015	QM/MM partial charges, binding pocket contours analysis and FEP calculation for designing potent inhibitors of HTLV- Protease: A <i>De novo</i> drug design approach	16.02
5.	DST, New Delhi	2011	2014	Computational Screening of CDK2 inhibitors by combined approach of pharmacophoric study, Quantum polarized ligand docking and molecular dynamics simulation study	18.95
6.	UGC (major) New Delhi	2011	2014	Shape and chemical feature based 3D-Pharmacophore Model generation, Virtual Screening and MESP studies to identify Potential Leads for Antifungal Azoles.	7.48
7.	AURF (UGC) with NIBI, Osaka	2009	2012	Pharmacophoric Analysis and designing of ATP competitive CDK 4 inhibitors.	4.00

Other Fund Received as Research Mentor: 5

S.No	Agency	Period		Project Title	Budget (INR)
		From	To		
1.	DST – WOS	2023	2025	Computational and Experimental studies on Identification of the potential Serotonin Transporter Gene (SERT) Antagonists for Autism Spectrum Disorder.	24,00,000

2.	ICMR - SRF	2023	2025	Molecular elucidation of regulatory proteins as drug target for identifying antimicrobial and ant biofilm inhibitors against spore forming bacteria	16,00,000
3.	RGNF	2016	2020	Theoretical studies to identify potential leads targeting the Oncoproteins of Human Papilloma virus	17,00,000
4.	CSIR SRF	2013	2014	Mechanistic Insights into HIV-1 integrase inhibition by strand transfer and LEDGF/p75 binding site inhibitors	3,33,880
5.	UGC – Dr. D.S. Kothari Post-Doctoral Fellow	2015	2016	Computational Drug Discovery	6,58,000

Distinctive Achievements/Awards

S.No	Awards/Honors	Granting Institution	Year	Description
1.	Appreciation Certificate	Alagappa University, Karaikudi	2020-21 to 2022-23	Recognizing his outstanding Academic and Research Excellence in acquiring the award & Project during academic years
2.	World Top 2% Most Influential Scientists list - 2023	Published by Stanford University, U.S.A	2023	Excellence in Research
3.	World Top 2% Most Influential Scientists list - 2022	Published by Stanford University, U.S.A	2022	Excellence in Research
4.	INSA Teacher Award-2022	Indian National Science Academy, New Delhi	2022	Inspiring students to take up careers in Science and Technology.
5.	Outstanding Researcher Award – 2022	Alagappa University, Karaikudi	2022	Excellence in Research
6.	Fellow of Royal Society of Chemistry	Royal Society of Chemistry, London, United Kingdom	2021	Outstanding contribution in the field of Molecular Modelling and Computer Aided Drug Design with Quantum chemistry applications.
7.	Fellow of Royal Society of	Royal Society of	2021	Extensive research involved in

	Biology	Biology, London, United Kingdom		the field of Biological Sciences.
8.	Member of Board of Governors	Biotech Research Society of India (BRSI), India	2021 - 2023	-
9.	Fellow of Academy of Sciences	The Academy of Sciences, Chennai, Tamil Nadu, India	2020	In recognition of the significant contribution for the Advancement of Science
10.	Vallal Alagappan Research Recognition Award	Alagappa University, Karaikudi.	2020	Contribution towards the enhancement of Research outcome of the university in the form of "h" index
11.	Biotech Research Society, India (BRSI) Fellow Award	Biotech Research Society, India	2018	Outstanding contribution to Structural Bioinformatics and Computer-Aided Drug Design.
12.	ICMR-Lala Ram Chand Kandhari Award	Indian Council of Medical Research (ICMR), New Delhi	2014	Outstanding contribution in the area of Sexually Transmitted Diseases
13.	Dr. P. Daisy Oration Award	Holy Cross College, Tiruchirappalli	2017	Outstanding contribution to the life-threatening diseases like Cancer and HIV
14.	Senior Scientist Award.	the Association of Biotechnology and Pharmacy (ABAP)	2017	Immense contribution in the field of Computational drug discovery and development of novel inhibitors for HIV/AIDS
15.	Elected Member of National Academy of Sciences, Allahabad, India (MNASc)	National Academy of Sciences, Allahabad, India (MNASc)	2017	-
16.	Elected Secretary-General of Bioinformatics and Drug Discovery Society (BIDDS)	Bioinformatics and Drug Discovery Society (BIDDS), Karaikudi	2017	-
17.	DST Fast Track grant for Young Scientist	Chemical Sciences	2010	Excellence in Research

Events Organized in Leading roles

Number of Seminars / Conferences / Workshops / Events organized: 26

Position	Programme	Duration	Institution
Co-Convenor	2nd International Conference cum workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" [ICSBCADD'2022] and 6th Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]	2022	Alagappa University, Karaikudi
Organizing Committee Member	INDO-US Symposium on Molecular Virology-2022	2022	IIT Mandi, Himachal Pradesh

Coordinator	One-day Radiation Awareness Program and Celebration of 125th year of Discovery of X-rays and radioactivity	2021	Alagappa University with IGCAR, Kalpakkam and IARP, Kalpakkam
Coordinator	Webinar titled "Jammu and Kashmir: Past, Present and Way Forward"		Alagappa University, Karaikudi
Organizing Secretary	Curtain Raiser and Outreach Programme "Science for Self Reliant India and Global Welfare" under the India International Science Festival (IISF-2020)	2020	Alagappa University, Karaikudi
Organizing Secretary	Special Lecture on 'History of Indian Science' under India International Science Festival, IISF-2020	2020	Alagappa University, Karaikudi
Co-Convenor	International Conference on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" [ICSBCADD'2019] and 3rd Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]	2019	Alagappa University, Karaikudi
Organizing Secretary	11th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2018 and 2nd Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]	2018	Alagappa University, Karaikudi
Organizing Committee Member	International Conference on Bioinformatics (INCOB) – 2018	2018	Jawaharlal Nehru University, New Delhi
Organizing Committee Member	10th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2018 and 1st Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]	2018	Alagappa University, Karaikudi
Organizing Secretary	9 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2014	2014	Alagappa University, Karaikudi
Organizing Committee Member	International Conference on Recent Trends in Biosciences (ICRTB) April, 2016	2016	Alagappa University, Karaikudi
Organizing Committee Member	8 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2016	2016	Alagappa University, Karaikudi
Organizing Committee Member	7 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2015	2015	Alagappa University, Karaikudi
Organizing Secretary	6 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2014	2014	Alagappa University, Karaikudi
Organizing Committee Member	5th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design" 2013	2013	Alagappa University, Karaikudi
Organizing Committee Member	4th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design" 2012	2012	Alagappa University, Karaikudi

Co-organizing Secretary	3rd National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design" 2011	2011	Alagappa University, Karaikudi
Convener	2nd National Workshop on "Application of Molecular Modeling and Structural Bioinformatics" 2010	2010	Alagappa University, Karaikudi
Organizing Secretary	Workshop on "Computer Aided Drug Design" 2009	2009	M. K Uni., Madurai
Organizing Secretary	Workshop on Systems Biology and its application 2008	2008	M. K Uni., Madurai
Organizing Secretary	Workshop on Bioinformatics Software's 2008	2008	M. K Uni., Madurai
Organizing Secretary	Workshop on System's Biology and Bioinformatics 2007	2007	M. K Uni., Madurai
Organizing Committee Member	Workshop on "Molecular Modelling and Pharmacoinformatics 2006	2006	NIPER, Mohali.
Organizing Committee Member	Workshop on "Pharmacoinformatics in Drug Design 2005	2005	NIPER, Mohali.
Organizing Committee Member	Workshop on Pharmacoinformatics: QSAR (2004	2004	NIPER, Mohali.

Events Participated

Number of Conferences / Seminars / Workshops: 95

Overseas Exposure / Visits				
S.No	Country	Purpose of visit	Year	Institution/Organization
1.	Switzerland	European Conference on Computation Biology (ECCB-2012), A 11th European Conference on Computational Biology	9 th -12 th September 2012	Swiss Institute of Bioinformatics, University of Basel, Switzerland
2.	Germany	Visit to European Molecular Biology Lab (EMBL)	13 th September 2012	European Molecular Biology Lab (EMBL)
3.	USA	Albany 2011, The 17th Conversation	14 th -18 th June 2011	University at Albany, New York, USA
4.	USA	Visit to Department of Chemistry and Structural Biology, and Computer Science lab	24 th -25 th June 2011	Stanford University, Stanford, California

5.	China	Invited talk at 5th Annual Congress of International Drug Discovery Science and Technology Conference (IDDST-2007)	7 th -13 th November, 2007	Xian, China
6.	China	Invited talk entitled “Drug Discovery Science and Technology Research”	2007	Xian Technical University and Xian Technology Park

Membership

Professional Bodies

S. No.	Membership Type	Organization name
1.	Life Member	Chemical Research Society of India (CRSI)
2.	Life Member	Protein Society (PS), India
3.	Life Member	Bioinformatics and Drug Discovery Society (BIDDS), India
4.	Life Member	The Biotech Research Society(BRSI), India
5.	Elected Life Member	The National Academy of Sciences (NASI), Allahabad, India
6.	Life Member	Society for Biological Chemist (SBC),
7.	Life Member	Indian Biophysical Society (IBS)
8.	Life Member	The Indian Science Congress Association (ISCA)
9.	Life Member	Society for Biotechnology, India
10.	Joint Secretary	Bioinformatics Forum, Allahabad
11.	Member	Trends on Theoretical Chemistry Biannual Conference
12.	Member	Indo-French Bioinformatics Meeting

Advisory Board

Year / Period	Name of the BoS / Administrative Committee / Academic Committee	Role
2020	“Innovations and Implementations of Drug Discovery Strategies in Rational Drug Design” published by <i>Springer Nature</i> in [ISBN 978-981-15-8936-2]	Edited a book
1 st January 2021 -31 st December 2023	Journal of Microbiology and Biotechnology (JMB)	Editorial Board member
2017 to till date	Journal of AIDS and HIV Infection (JAHI)	Editorial Board member
1 st April, 2016-31 st March, 2019	Journal of Microbiology and Biotechnology (JMB)	Editorial Board member
4th issue entitled ‘Computer Aided Drug Design’ of BIOBYTES, Open Access Newsletter of Biotechnology Information System (BTIS), Department of Biotechnology (DBT), Government of India.		<u>Guest Editor</u>
Medicinal Chemistry, Bentham Science Publishers		Guest Editor
Special issue of SBCADD’2019 in the Journal of “Current Computer-Aided Drug Design” published by Bentham Science		Guest Editor

Depiction on the resistance developed in HIV patients experienced with the drugs of HIV” will be published by Elsevier Publishers – 2022	Editing a book
Application of IDH2 inhibitors to reverse Drug Resistance in cancer Chemotherapy will be published by Elsevier Publishers- 2022.	Editing a book

Academic Bodies in Other Institutes/ Universities		
Year / Period	Name of the BoS / Administrative Committee / Academic Committee	Role
2023 - 2025	Biotech Research Society of India (BRSI),	Member of Board of Governors
2021 - 2023	Biotech Research Society of India (BRSI),	Member of Board of Governors
2018 – 2020	Alagappa University, Karaikudi	Member of Board of Studies of Bioinformatics
2017- Till date	Alagappa University, Karaikudi	Secretary-General of Bioinformatics and Drug Discovery Society (BIDDS)
2017- Till date	National Academy of Sciences, Allahabad, India (NASI)	Elected Member of National Academy of Sciences
2016	Periyar University, Salem	Member of Board of Studies in Bioinformatics
2016	Bharthidasan University, Trichy, Tamilnadu	Chairman of the University Rank Examination Question Paper Setting for M.Sc. Bioinformatics
2010-2013	Alagappa University, Karaikudi	Member of Board of Studies of Bioinformatics
2009	Pondicherry University, April	Member of Board of Central Evaluation in Bioinformatics
Nov. 2010	Pondicherry University	External Member of programme Committee in Bioinformatics
2013 - 2016	Alagappa University	Member Board of Studies of UGC Innovative programme on “Structural Pharmacogenomics”
2009 - 2012	Lady Dock College, Madurai Kamaraj University, Madurai.	Member of board of Studies in Advance diploma in Molecular Modeling sponsored by DBT, New Delhi,

Ph.D. Thesis Guided

1. No. of PhD Thesis evaluated : 52
2. No. of PhD Public Viva Voce Examination conducted : 32

S. No	Name of the Scholar	Title of the Thesis	Year of Completion
1	Dr. Sunil Kumar Tripathi	Exploring the selectivity of cyclin-dependent kinase-2 (CDK2) protein and its inhibitors towards therapeutic target for Cancer	Completed
2	Dr. Chandrabose Selvaraj	Structural insights into SrtA-LPXTG blockers and enhancement of microbial inhibition through beta-cyclodextrin inclusion complex	Completed
3	Dr. Karnati Konda Reddy	Mechanistic Insights into HIV-1 integrase inhibition by strand transfer and LEDGF/p75 binding site inhibitors	Completed
4	Dr. Suryanarayanan Venkatesan	Theoretical and experimental studies on histone acetyltransferases as epigenetic target for cancer therapy	Completed
5	Dr. Vijaya Prabhu Sitrarasu	Computational investigation of allosteric modulators for Group I metabotropic glutamate receptors against neurodegenerative diseases	Completed
6	Umesh Panwar	Mechanistic insights of HIV-1 Integrase-Human LEDGF/p75 interaction and designing of therapeutics against viral infection	Completed
7	Anuraj NS	Whole genome sequencing of Biosurfactant producing bacteria using next generation sequencing	Completed
8	M. Aarthy	Theoretical studies to identify potential leads targeting the Oncoproteins of Human Papilloma virus	Completed
9	Ishwar Chandra	Theoretical and structural analysis on HIV attachment and protease inhibitors	Completed
10	Chirasmitta Nayak	Systems biology and structural bioinformatics study on Glioblastoma multiforme (GBM)	Thesis submitted
11	Mohd. Aqueel Khan	Theoretical experimental studies on HIV proteins to develop the novel therapeutic agents	On-going
12	Ms. R. Abhirami	Molecular elucidation of regulatory proteins as drug target for identifying antimicrobial and antibiofilm inhibitors against spore forming bacteria	On-going
13	M. Arun Pravin	Exploration of the Flavivirus ideal drug targets that facilitate cleavage of Key host proteins for the immune evasion mechanism	On-going
14	Mr. Sushil Kumar	Computational approaches for investigating the dengue Entry Level Proteins and molecular insights of inhibition mechanism	On-going
15	Ms. O. Rudhra	Computational and Experimental studies on Identification of the potential Serotonin Transporter Gene (SERT) Antagonists for Autism Spectrum Disorder	On-going
16	Ms. Anushka Bhardwaj	Next Generation sequencing of natural therapeutic products producing bacteria and computational	On-going

		screening against various drug targets	
17	Ms. G. Rubha Shri	Exploring the enzymes involved in HTLV-1 cell communication and replication mechanism: A Computational Drug Discovery Approach	On-going
18	Mrs. Khushboo Sharma	Whole Genome Sequencing and Structural Bioinformatics approach towards Plasticizer-Degrading Microbes	On-going
19	Mrs. Arshiya Khan	Whole Genome Sequencing and Structural Bioinformatics approach towards Dye-Degrading Bacteria	On-going

List of Research Articles / Recent Publications : 215

S. No	Authors/Title of the paper/Journal	Impact Factor
1.	Gupta, P., Panwar, U., & Singh, S.K. , 2024. Novel scaffolds identification against Mpro of SARS-CoV-2 using shape based screening and molecular simulation methods. <i>Chemical Physics Impact</i> , p.100496.	IF- 2.2
2.	Sharma, K., Panwar, U., Madhavi, M., Joshi, I., Chopra, I., Soni, L., Khan, A., Bhrdwaj, A., Parihar, A. S., Mohan, V. P., Prajapati, L., Sharma, R., Agrawal, S., Hussain, T., Nayariseri, A., & Singh, S.K., 2024. Unveiling the ESR1 Conformational Stability and Screening Potent Inhibitors for Breast Cancer	IF-8.0
3.	Shiammala, P. N., Duraimutharasan, N. K. B., Vaseeharan, B., Alothaim, A. S., Al-Malki, E. S., Snekaa, B., Safi, S. Z., Singh, S.K. , Velmurugan, D., & Selvaraj, C., 2023. Exploring the artificial intelligence and machine learning models in the context of drug design difficulties and future potential for the pharmaceutical sectors. <i>Methods</i> , 219, 82–94.	IF- 4.8
4.	Nayariseri, A., & Singh, S.K. , 2023. Genome analysis of biosurfactant producing bacterium, Bacillus tequilensis. <i>Plos One</i> , 18(6), e0285994.	IF-3.7
5.	Selvaraj, C., Dinesh, D. C., Pedone, E. M., Alothaim, A. S., Vijayakumar, R., Rudhra, O., & Singh, S. K.* (2023). SARS-CoV-2 ORF8 dimerization and binding mode analysis with class I MHC: computational approaches to identify COVID-19 inhibitors. <i>Briefings in Functional Genomics</i> , elac046.	IF-4
6.	Bhrdwaj, A., Abdalla, M., Pande, A., Madhavi, M., Chopra, I., Soni, L., ... & Singh, S. K. (2023). Structure-Based Virtual Screening, Molecular Docking, Molecular Dynamics Simulation of EGFR for the Clinical Treatment of Glioblastoma. <i>Applied Biochemistry and Biotechnology</i> , 1-26.	IF-3
7.	Nayariseri, A., Bhrdwaj, A., Khan, A., Sharma, K., Shaheen, U., Selvaraj, C., ... & Singh, S. K. Singh, S. K. * (2023). Promoter–motif extraction from co-regulated genes and their relevance to co-expression using E. coli as a model. <i>Briefings in Functional Genomics</i> , elac043.	IF-4
8.	Murali, A., Kumar, S., Akshaya, S., & Singh, S. K.* (2023). Drug repurposing toward the inhibition of RNA-dependent RNA polymerase of various flaviviruses through computational study. <i>Journal of Cellular Biochemistry</i> , 124(1), 127-145.	IF-4
9.	Selvaraj, C., Panwar, U., Ramalingam, K. R., Vijayakumar, R., & Singh, S. K.* (2022). Exploring the macromolecules for secretory pathway in cancer disease. <i>Advances in Protein Chemistry and Structural Biology</i> , 133, 55-83.	-
10.	Selvaraj, C., Ramalingam, K. R., Velmurugan, D., & Singh, S. K. * (2022). Transcriptional regulatory mechanisms and signaling networks in cancer. <i>Advances in Protein Chemistry and Structural Biology</i> , 134, 1-20.	-

11.	Khan, M. A., & Singh, S.K.* (2022). Atom-based 3D-QSAR and DFT analysis of 5-substituted 2-acylaminothiazole derivatives as HIV-1 latency-reversing agents. <i>Journal of biomolecular structure & dynamics</i> , pp.1-16.	IF-4.4
12.	Selvaraj, C., Pravin, M. A., Alhoqail, W. A., Nayarisseri, A., & Singh, S. K.* (2022). Intrinsically disordered proteins in viral pathogenesis and infections. <i>Advances in protein chemistry and structural biology</i> , 132, 221–242.	
13.	Aarthy, M., Muthuramalingam, P., Ramesh, M., & Singh, S.K.* (2022). Unraveling the multi-targeted curative potential of bioactive molecules against cervical cancer through integrated omics and systems pharmacology approach. <i>Scientific Reports</i> , 12, 14245.	IF-4.6
14.	Jeyakumar, M., Sathya, S., Gandhi, S., Tharra, P., Aarthy, M., Balan, D. J., ... Singh, S. K. & Devi, K. P. (2022). α -bisabolol β -D-fucopyranoside inhibits β -amyloid (A β) 25–35 induced oxidative stress in Neuro-2a cells via antioxidant approaches. <i>Process Biochemistry</i> , 121, 493-503.	IF-4.4
15.	Nayak, C., & Singh, S. K*. (2022). Integrated Transcriptome Profiling Identifies Prognostic Hub Genes as Therapeutic Targets of Glioblastoma: Evidenced by Bioinformatics Analysis. <i>ACS omega</i> , 7(26), 22531–22550.	IF-4.1
16.	Selvaraj, C., Shri, G. R., Vijayakumar, R., Alothaim, A. S., Ramya, S., & Singh, S. K*. (2022). Viral hijacking mechanism in humans through protein–protein interactions. <i>Advances in Protein Chemistry and Structural Biology</i> .	-
17.	Selvaraj, C., Rudhra, O., Alothaim, AS., Alkhanani, M., and Singh, S.K*. (2022). Structure and Chemistry of Enzymatic Active Sites that play a role in the Switch and Conformation Mechanism. <i>Advances in Protein Chemistry and Structural Biology</i> , 130, 59-83.	-
18.	Yadav, M., Abdalla, M., Madhavi, M., Chopra, I., Bhrdwaj, A., Soni, L., ... & Singh, S. K*. (2022). Structure-Based Virtual Screening, Molecular Docking, Molecular Dynamics Simulation and Pharmacokinetic modelling of Cyclooxygenase-2 (COX-2) inhibitor for the clinical treatment of Colorectal Cancer. <i>Molecular Simulation</i> , 1-21.	IF-2.1
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	<i>Advancement towards Therapeutic Drug Delivery (Part II)</i> , 151.
197.	Selvaraj, C., Singh, S. K* . (2021). Eco-friendly Microbial Biopolymers: Recent Development, Biodegradation, and Applications. In <i>Microbial Polymers</i> (pp. 547-577). Springer, Singapore.
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215.	Selvaraj, C., Tripathi, S.K. and Singh, S.K* . Active Sites prediction on molecular modelling studies, <i>Recent Trends in Computational Biology and Computational Statistics Applied in Biotechnology and Bioinformatics</i> , 2011 New India Publishing Agency.

Resource persons in various capacities

National Conferences	:	52
International Conferences	:	16
Invited Lectures	:	68

S. No.	Title of Lecture	Short Term Course/ Conference/Organization	Date	Organization
1.	AI/ML Based Drug Design and its importance in Modern Drug Development	International Conference on Structural Biology and Drug Discovery (ICSBDD – 2024)	16 th – 17 th February 2024	Sengamal Thayaar Educational trust Women's College, Mannargudi, TN
2.	AI/ML based drug design of contribution of MDS in drug development	Short-Term-Course (STC) on "Transforming Healthcare with AI-Driven Drug Discovery", held at IIT-BHU	18th – 22nd December 2023	IIT-BHU, Varanasi
3.	Structural interpretation of Virus and Human protein Interactions: A Computer Aided Drug Design Studies	International Conference on New Horizons in Biotechnology (NHBT-2023)	26th-29 th November 2023	CSIR – National Institute for Interdisciplinary Science and Technology (NIIST), Trivandrum, Kerala
4.	Structural Elucidation of Virus and Human	Conference on Structural Biology and Drug	09.10.2023	Department of Biotechnology, SRM
5.	Virus and Human Interaction: A Computational Drug	Short-Term Course on Computer-Aided Drug Design and Structural	16.03.2023	IIT BHU, Varanasi, U.P

	Discovery approach and Demo on Pharmacophore and QSAR in Drug Discovery	Bioinformatics (CADD SB-2023) March 13-17, 2023		
6.	Virus and Human Interaction: A Computational Drug Discovery approach	Conference on Structural Bioinformatics and Computer Aided Drug Design	10.11. 2022	ILS Bhubaneswar, Odisha
7.	Virus and Human Interaction: A Computational Drug Discovery approach	International Conference on Computational Biology and bioinformatics	5.11.2022	National College, Trichy
8.	Computational investigations on SARS-CoV-2 Drug Targets to design potential Drugs for CoVID-19	Recent Trends in Macromolecular Structure and Functions, Marine Biotechnology and Bioinformatics International Symposium on (ISRTMSF2022)	6 th Oct 2022	AMET University, Chennai
9.	Designing of Responsive Agent to eradicate HIV: A Computational Drug Discovery Approach	SERB Sponsored Workshop on “Hands-On Training on Computer Aided Drug Design and Discovery Tools” from	11 th - 17 th July, 2022	Shree S. K. Patel College of Pharmaceutical Education and Research, Ganpat University, Gujarat
10.	Learning-How to Learn	National Programs For Orientation of Science Teachers	16 th -17 th April, 2022	Rajalakshmi Institute of Technology, Chennai
11.	Thematic Lecture	ACT NEXT 2021	17 th March, 2022	Department of Physics & IQAC, Alagappa University, Karaikudi
12.	Molecular level Comprehending of HIV Drug Targets for the identification of potential Drugs: A Computational Drug Discovery Approach	Recent Trends of Computational Biology in Basic & Translational Research	10 th March, 2022	ACTREC, Navi Mumbai, Maharashtra
13.	Evaluation of SARS-CoV-2 drug targets to	INDO-US Symposium on Molecular Virology-2022	17 th March, 2022	IIT-Mandi, Himachal Pradesh
14.	Advancement in Computational Drug Discovery and its application	Refresher Course – Life Sciences	22 nd November, 2021	UGC-Human Resource Development Centre, Sant Gadge Baba Amravati University, Maharashtra
15.	Molecular level Insights of SARS-CoV-2 Drug Targets for the identification of COVID-19 Inhibitors	Refresher Course – Life Sciences	22 nd November, 2021	UGC-Human Resource Development Centre, Sant Gadge Baba Amravati University, Maharashtra 444602

16.	SARS-CoV-2 Drug Targets for COVID-19 Inhibitors	NCCBDD-2021	11 th -12 th September , 2021	I-DAPT hub foundation IIT-BHU, Varanasi BIDDS
17.	Computer Aided Drug Design tools	Computer Aided Drug Design and Protein Analysis	February 22 nd -26 th , 2021	IIT-BHU, Varanasi, Uttar Pradesh
18.	Advancement in Computational Drug Discovery	E-learning program on Bioinformatics	21 st May, 2020	Dept. Of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu
19.	Hands on sessions on the various Computer Aided Drug Design tools	Computer Aided Drug Design and Protein Analysis Online Short-term Course	February 22-26, 2021	IIT BHU
20.	Advancement in computational Drug Discovery	E-learning program on Bioinformatics as Cartographic tool in Drug Discovery (Webinar)	May 21 st , 2020	Dept. Of Bioinformatics, Alagappa University, Karaikudi
21.	Webinar cum hands on training	Computational Approaches for Anti-microbial Drug	21 st August, 2020	Department of Biotechnology, Karpagam Academy of Higher Education
22.	Keynote Lecture	Emerging Trends in Biotechnological Advancements: Challenges and Prospects in Tackling Human Diseases	13 th – 17 th July, 2020	Department of Biotechnology, NIT, Warangal
23.	Keynote Lecture	Research Environment during the Post Covid Era” in the FDP-Webinar Series III	13 th – 18 th July, 2020	Holy Cross College, Tiruchirapalli, Tamil Nadu
24.	Designing of responsive agents using in silico strategies : The way to eradicate HIV Infections	NHBT-2019 : International Conference On New Horizons In Biotechnology, Trivandrum, Kerala	20 th -24 th November, 2019	The Biotech Research Society, India
25.	Design of novel inhibitors to combat viral infection : A rational drug design approach	National Conference on Emerging Trends In Disease Model Systems - 2019	25 th -27 th March , 2019	NCCS, Pune
26.	Computational drug discovery approaches	Invited Lecture	23 rd January , 2019	Bishop Heber College, Trichy
27.	Molecular insights into the binding site for developing effective drugs	National Conference on Advanced Bio-Chem Development – 2018 (ABCD)	18 th -19 th September , 2018	Sri Sarada Niketan College for Women, Karaikudi.
28.	Computational drug discovery :Designing novel inhibitors for treating HIV/ AIDS	“International Conference on Innovations in Pharma and Biopharma Industry : Challenges and Opportunities for Academy and Industry”	21 st December , 2017	University of Hyderabad, Hyderabad

29.	Theoretical studies on HIV integrase inhibitors.	Invited Talk in National Conference on Innovations in Biotechnology (NCIB-2017)	14 th -15 th December , 2017	Madurai Kamaraj University, Madurai
30.	<i>In silico</i> studies on HIV IN, Protease and Reverse Transcriptase.	International Conference on Innovations and Challenges in Biomedical Sciences Research	12 th -14 th December , 2017	Holy Cross, Trichy
31.	Computational drug discovery : An avenue for targeting the protein-protein interaction between HIV-1 integrase and LEDGF/p75	Invited Talk in National Conference on Protein Structure and Dynamics in Health and Agriculture	3 rd and 04 th , November 2017	Jamia Milia Islamia University, New Delhi
32.	Structural Insights in finding out the HIV Inhibitors	Invited Lecture to deliver talk in Conference "Novel Technologies on Natural Products for Mosquito and Disease Control"	23rd and 24th February, 2017	K.S. Rangasamy College of Arts and Science, Tiruchengode, Namakkal, Tamil Nadu
33.	Computers in Drug Discovery	Invited for delivering a plenary lecture at Department of Information Technology	24 th August, 2016	Dr. Umayal Ramanathan College for Women, Karaikudi
34.	Importance and Contribution of CADD and Molecular Modelling in HIV inhibitors	Occasion of Signing of MoUs	7 th March, 2016	Periyar University, Salem
35.	Theoretical studies on HIV-1 Integrase Inhibition by Strand Transfer and LEDGF/P75 Binding site Inhibitors	Annual meeting of the Indian Biophysical Society	9 th February, 2016	Indian Biophysical Society, Bangalore
36.	Molecular Modeling and CADD in current Scenario	Remedial Coaching Class	22 nd January, 2016.	Alagappa University
37.	Impact of Computer aided drug design and Molecular modeling in current drug discovery	Recent developments in Medical Biotechnology and Structure based Drug designing	6 th -7 th December, 2015	Indian Institute of technology, Guwahati
38.	Mechanistic insights on HIV-1 integrase inhibition by strand transfer and LEDGF/p75 binding site inhibitors: a computational approach	Recent developments in Medical Biotechnology and Structure based Drug designing	7 th December, 2015	Indian Institute of technology, Guwahati
39.	Molecular Modeling and Dynamics Studies of HIV & HTLV Inhibitors	Symposium cum Workshop on "Advances in Computational Biology and Computer Aided Drug Design" during	24 th -26 th , June, 2015	BSBE, Indian Institute of Technology Guwahati

40.	Comprehensive Approach of Biotechnological Applications	Faculty Development Programme	16 th -29 th April, 2015	BIT, Anna University, Trichy.
41.	Current Topics in CADD	Key note address at National seminar on Genomics and Proteomics: A Computational Approach	6 th March, 2015.	Lady Dock College, Madurai
42.	Contribution of Computer Aided Drug Design in Current Drug Discovery	Resource person & delivered a key note lecture at one day workshop on "Molecular Modeling & Biopharmaceutical drug design for biotechnology researchers (MMBDDBR, 2015)	5 th March, 2015	Periyar University, Salem
43.	Theoretical Studies on HIV Integrase Inhibitors	Plenary lecture at National seminar on Bioinformatics (NSB'15)	28 th – 29 th January, 2015.	Bharathidasan University, Trichy.
44.	"Contribution of Computer Aided Drug Design in Current Drug Discovery"	Invited lecture at DST-PURSE sponsored One Day Lecture Workshop on "Application of Computational Chemistry and Biology"	3 rd March, 2015.	MaduariKamaraj University, Madurai on
45.	QM/MM studies on HIV-Integrase Strand Transfer Inhibitors	Recent Strategies in Drug Discovery - III	25 th - 27 th , September 2014	PSG college of Arts and Science, Coimbatore
46.	Computer aided drug design and its importance in current drug discovery	National Conference on Bioengineering and Biotechnology An Industrial Perspective	16 th -17 th October, 2014	AMITY, Lucknow
47.	Theoretical studies on CDK2 and HIV-Integrase inhibitors	National Conference on Society for Biotechnologies	November, 2013	S. G. B. Amravati University
48.	Currents trends in Pharmacoinformatics	Workshop on Molecular Modeling and Drug Design	14 th to 20 th July 2013	PSG college Coimbatore
49.	The molecular level energy calculation and Molecular dynamics studies on structurally similar HTLV and HIV protease enzymes using HIV-PR inhibitors	IWBIO-2013	18 th -20 th Mar, 2013	Granada, Spain
50.	A Theoretical Study of CDK2 Protein-Ligand Interactions through QM/MM interaction energy approach	Theoretical Chemistry Symposium	20 th December, 2012	IIT, Ghawhati
51.	Molecular Docking of Small Molecules	National workshop on "Molecular Docking of Small Molecules	27 th to 29 th January 2011	Lady Dock College, Madurai

52.	CADD in Pharmaceutical Development	International year of chemistry Celebration	October, 2011	Gandhigram University, Dindigul
53.	Pharmacophoric study and QSAR model on Anti-Fungal Azoles	National Seminar on Advances in Bioinformatics	08 th February, 2011	Holy Cross College, Trichy
54.	<i>In-Silico</i> screening in Drug Discovery	UGC sponsored academic staff college refresher course	03 rd to 18 th December 2010	Bhartidasan University, Trichy
55.	Ligand and Structure based Drug Design	UGC sponsored academic staff college refresher course	March, 2010	Amarawati University, Maharashtra
56.	Molecular Docking Studies on Antifungal Azoles	Genomics workshop	November, 2008	ILS Bhubaneswar
57.	Application of QSAR in Pharmaceutical Industry	CADD workshop	October, 2008	Pondicherry University
58.	CADD in pharmaceutical industry	Workshop on Industrial Bioinformatics	February, 2008	Bharathiyar University Coimbatore
59.	Over view of Molecular Modeling and Computer Aided Drug Design	Bioinformatics workshop	29 th August, 2007	JALMA Leprosy Institute (ICMR Lab), Agra
60.	“Computer Aided Drug Design”	Presentation in CTDDR	7 th February, 2007	CDRI Lucknow
61.	CADD and Bioinformatics	International Seminar on Bioinformatics	November, 2007	L. D. College, Madurai
62.	Bioinformatics in Life Sciences	Presentation at Academic Staff College	September, 2006	MKU, Madurai
63.	QPLD analysis on HIV-integrase inhibitors	National Workshop on “Recent trends in Bioinformatics”	11 th - 12 th July, 2007	School of Biotechnology, MKU, Madurai
64.	Pharmacophoric Studies on ACE inhibitors	Workshop on “Computer Aided Drug Design” in association with SCHRODINGER, USA.	06 th - 08 th March, 2007	School of Biotechnology, MKU, Madurai
65.	Challenges and Solution in CADD and Molecular Modeling	Silicon Graphics Technology Submit 2006	Dec. 2006	Chennai
66.	3D-QSAR CoMFA and CoMSIA study on Benzodipyrazoles as CDK2 Inhibitors	Workshop on Pharmaco-informatics: QSAR	01 st - 03 rd March, 2006	NIPER, Mohali, India
67.	QSAR studies on indenopyrazole derivatives	Indo-French Bioinformatics Meeting	12 th - 14 th June, 2006	NCBS, Bangalore
68.	Virtual screening on CDK inhibitors	Workshop on Systems Biology and its application	06 th - 08 th September, 2006	School of Biotechnology, MKU, Madurai
69.	3D-QSAR studies on	National Workshop on	14 th - 16 th	(NIPER) Mohali, Punjab.

	benzodipyrazole series of CDK inhibitors	“Pharmacoinformatics in Drug Design”	April 2005	
70.	QSAR studies on indenopyrazole derivatives	9th biannual discussion meeting in theoretical Chemistry	9 th – 12 th December 2005	BARC, Mumbai
71.	QSAR studies on indenopyrazole derivatives	9 th biannual discussion meeting in Theoretical Chemistry	09 th – 12 th , December, 2005	BARC, Mumbai
72.	Quantum Pharmacological study on HIV-1RT Inhibitors	7 th biannual discussion meeting on Theoretical Chemistry	January. 2004	IIT Kanpur
73.	Pharmacophoric features of HIV-1RT inhibitors	8 th biannual discussion meeting in Theoretical Chemistry	17 th -19 th , January, 2003	IACS, Jhadavpur, Kolkata

Dr. Sanjeev Kumar Singh
(Professor)