



Dr. Sanjeev Kumar Singh
Professor

Contact

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Academic Qualifications:

Year	Degree	Subject	University/Institute
2004	Ph. D.	Applied Chemistry	CSJM University, Kanpur
2000	M. Sc.	Life Sciences	Institute of Life Sciences, CSJM University, Kanpur
1998	B. Sc.	Zoology, Botany, Chemistry	Christ Church College, CSJM University, Kanpur

Teaching Experience and Research experience: 20 Years

Designation	Name of Employer	Period		No. of Years /Months
		From	To	
Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	20 th March, 2015	Continue	6 years & 4 months
Associate Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	20 th March, 2012	19 th March, 2015	3 years
Reader	Dept. of Bioinformatics Alagappa University Karaikudi	20 th March, 2009	19 th March, 2012	3 years
Lecturer	CoE in Bioinformatics, School of Biotechnology, Madurai Kamaraj University	31 st March, 2006	19 th March, 2009	3 years

RA/Scientist-II	Pharmacoinformatics Division, NIPER, Mohali	June, 2004	30 March, 2006	1 year 9 months
Senior Research Fellow	Dept. of Chemistry, IET, CSJM University, Kanpur	18 Nov, 2002	May, 2004	1 year 6 months
Junior Research Fellow	Dept. of Chemistry, IET, CSJM University, Kanpur	18 Nov, 2000	17 Nov, 2002	2 years

Additional Responsibilities

Responsibility in University/Community Services	
1.	Nodal Officer for the “ India International Science Festival (IISF) 2020 ” organized together CSIR and CSIR-National Institute of Science, Technology and Development studies (NISTADS) under the science & technology-related Ministries and (Govt. of India) from Alagappa University.
2.	Coordinator for Rashtriya Uchchar Shiksha Abhiyan (RUSA 2.0) sponsored by TN and MHRD, Govt. of India with the amount of Rs. 100 Crores for the Quality enhancement in Teaching & Research at Alagappa University (Feb. 2019 onwards).
3.	Nodal Officer for the “ Ek Bharat Shreshta Bharat ” Scheme under the Ministry of Human Resource and Development (Govt. of India) from Alagappa University.
4.	Nodal Officer for Niti Aayog – Grant in aid schemes for CSOs/NGOs/VOs in State Government at Alagappa University
5.	Special Officer (Projects) at Alagappa University from Dec 2017 – Jan 2019.
6.	Deputy Coordinator for Rashtriya Uchchar Shiksha Abhiyan (RUSA) at Alagappa University (Sep 2017- Dec 2019)
7.	Secretary General – Bioinformatics and Drug Discovery Society (BIDDS), Feb. 2017 onwards.
8.	Deputy Coordinator , DST-FIST Program (Level-I) at Department of Bioinformatics, Alagappa University (2017 onwards).
9.	Department Coordinator of UGC-NAAC at Department of Bioinformatics, Alagappa University (2016 - 2019).
10.	Liaison officer at Alagappa University (2016 - 2019)
11.	Involved in the activity of “Village Placement program” conducted by Alagappa University.
Responsibility in Corporate Life	
12.	Invited for lecture and training in personality development at Department of Bank Management, Alagappa University, karaikudi.
13.	Invited for lecture and training in personality development at Bharthidasan University, Trichy.
Nominated as the inspection team member for affiliation DDE Centre’s	
14.	Kurinji College of Arts and Science, Gateway for Entrepreneurship and Management Studies Trust, Trichy.
15.	Dharmapuram Adhinam Arts College, Sree Radhaa Krishna Educational Trust, Mayiladuthurai.
16.	Shri APM Trust, Thuraiyur, Trichy

Areas of Research

Research Expertise: Structural bioinformatics and computer aided drug designing.

Research Fields:

- **Viroinformatics** : Advanced computational 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) and pancreatic lipase.

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	Ph.D.	08	05
	Post Doc	03	01
	M.Phil.	09	-
Project	PG	49	-
	UG / Others	18	-

Publications

International Journals	National Journals	Others
163	05	Books: 1 Chapters: 24 Reviews: 10

Cumulative Impact Factor (as per JCR): 464.51

h-index : 28

i10 index : 89

Total Citations : 2506

<https://scholar.google.co.in/citations?user=y7QuV9QAAAAJ&hl=en>

RESEARCH PROJECTS CARRIED OUT AS PI/ CO-PI

S. No	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
Completed Projects					
1.	MHRD-RUSA 2.0	2018	2021	Mechanistic insights to understand the virus-host interaction and the identification of next-generation drugs to combat viral infections	45.00
2.	MHRD, SPARC	2019	2022	Biophysics of Zika virus envelope protein, membrane fusion and inhibitor discovery	97.23
3.	DBT, New Delhi	2016	2019	In-Silico screening, theoretical calculation and in vitro studies for development of potential HIV1-PR inhibitors	19.51
4.	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
5.	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
6.	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
7.	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
8.	AURF (UGC) with NIBI, Osaka	2009	2012	Pharmacophoric Analysis and designing of ATP competitive CDK 4 inhibitors.	4.00
Ongoing Projects					
9.	Tamil Nadu – Higher Education Department	2020	2023	Scheme for Alternative Strategy to antibiotics in bacterial disease management at Alagappa University (PI)	100.00

10.	Tamil Nadu State Council for Higher Education (TANSCHHE), 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	20.16
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PROJECTS IN REVIEW PROCESS

S.NO.	Project Title	Funding Agency	Budget (Rs. In lakhs)	In Process
1.	Drug discovery platform against <i>Leishmania donovani</i> using integrated computational and experimental approaches	DST-SERB, New Delhi	50.00	Under review process

Note: Budget must be rounded to two decimal places

Distinctive Achievements / Awards

S.No	Award	Organization	Field/Work awarded	Year of Award
1.	Fellow of Royal Society of Chemistry	Royal Society of Chemistry, London, United Kingdom	For the outstanding contribution in the field of Molecular Modeling and Computer Aided Drug Design with Quantum chemistry application.	2021
2.	Fellow of Royal Society of Biology	Royal Society of Biology, London, United Kingdom	For the extensive involvement in the field of Biological Sciences with the support of theoretical concepts and techniques	2021
3.	ICMR-Lala Ram Chand Kandhari Award	Indian council of medical research (ICMR)	For the outstanding contribution in the area of Sexually Transmitted Diseases	2014
4.	Elected as a Member of BOARD OF GOVERNORS	Biotech Research Society of India (BRSI), India.	-	2021-2023
5.	Fellow of Academy of Sciences	The Academy of Sciences, Chennai, Tamil Nadu, India.	Computataional analysis on the lethal drug targets	2020
6.	Biotech Research Society, India (BRSI) Fellow Award	Biotech Research Society, India	For the outstanding contribution in Structural Bioinformatics and Computer-Aided Drug Design.	2018
7.	Alagappa Appreciation Award	Alagappa University	Appreciation award for ICMR-Lala Ram Chand Kandhari Award	2018

8.	Elected Member for The National Academy of Sciences, Allahabad, India (MNASc)	The National Academy of Sciences, Allahabad, India (MNASc)	-	2017
9.	Senior Scientist Award	Association of Biotechnology and Pharmacy (ABAP)	For immense contribution in the field of computational drug discovery and development of novel inhibitors for HIV/AIDS.	2017
10.	Dr. P. Daisy Oration Award	Holy Cross College, Tiruchirappalli	For the outstanding contribution in the life-threatening diseases like Cancer and HIV.	2017
11.	Indian Council of Medical Research (ICMR) Travel Award	ICMR	Paper Presentation in ECCB-12 in Basel, Switzerland.	2012
12.	Department of Science and Technology (DST) Travel Award	DST,	Paper Presentation in Albany, USA	2011
13.	DST Fast Track grant for Young Scientist-2010 in Chemical Sciences.	DST,	Chemical Sciences	2010
14.	Department of Biotechnology (DBT) Travel Award	DBT	Paper Presentation in IDDST-2007 in Xian, China	2007

Events organized in leading roles

Number of Seminars / Conferences / Workshops / Events organized: 24

S. No	Designation	Title	Organized at	Sponsors
1.	Coordinator	One day Radiation Awareness Program and Celebration of 125th year of Discovery of X-rays and radioactivity	Alagappa University with IGCAR, Kalpakkam and IARP, Kalpakkam	Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam and Indian Association for Radiation Protection (IARP), Kalpakkam
2.	Coordinator	Webinar titled "Jammu and Kashmir: Past, Present and Way Forward"	Alagappa University,	MHRD, Govt. of

			Karaikudi	India
3.	Organizing Secretary	Curtain Raiser and Outreach Programme "Science for Self Reliant India and Global Welfare" under the India International Science Festival (IISF-2020)	Alagappa University, Karaikudi	Alagappa University, Karaikudi
4.	Organizing Secretary	Special Lecture on 'History of Indian Science' under India International Science Festival, IISF-2020	Alagappa University, Karaikudi	Alagappa University, Karaikudi
5.	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]	Alagappa University, Karaikudi	Alagappa University, RUSA 2.0, DST-PURSE & SERB, DBT, ICMR, TNSCT, CSIR
6.	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]	Alagappa University, Karaikudi	Alagappa University, RUSA 2.0, DST-PURSE & SERB, CSIR.
7.	Organizing Committee Member	International Conference on Bioinformatics (INCOB) – 2018	Jawaharlal Nehru University, New Delhi	JNU, IIITD, DBT, DST-PURSE, ISCB, Apbians, PRTF, agrigenome, APBioNet
8.	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]	Alagappa University, Karaikudi	DBT, CSIR, ICMR, DST & Alagappa University
9.	Organizing Secretary	9 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2014	Alagappa University, Karaikudi	ICMR & Alagappa University
10.	Organizing Committee Member	International Conference on Recent Trends in Biosciences (ICRTB) April, 2016	Alagappa University, Karaikudi	Alagappa University
11.	Organizing Committee Member	8 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2016	Alagappa University, Karaikudi	DBT & Alagappa University
12.	Organizing Committee Member	7 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2015	Alagappa University, Karaikudi	DBT, DST, & CSIR
13.	Organizing Secretary	6 th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics	Alagappa University,	DBT & Alagappa

		and Computer Aided Drug Design" 2014	Karaikudi	University
14.	Organizing Committee Member	5th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design" 2013	Alagappa University, Karaikudi	DBT & Alagappa University
15.	Organizing Committee Member	4th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design" 2012	Alagappa University, Karaikudi	DBT & Alagappa University
16.	Co-organizing Secretary	3rd National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design" 2011	Alagappa University, Karaikudi	DBT & Alagappa University
17.	Convener	2nd National Workshop on "Application of Molecular Modeling and Structural Bioinformatics" 2010	Alagappa University, Karaikudi	DBT & Alagappa University
18.	Organizing Secretary	Workshop on "Computer Aided Drug Design" 2009	M. K Uni., Madurai	DBT & MKU
19.	Organizing Secretary	Workshop on Systems Biology and its application 2008	M. K Uni., Madurai	DBT & MKU
20.	Organizing Secretary	Workshop on Bioinformatics Software's 2008	M. K Uni., Madurai	DBT & MKU
21.	Organizing Secretary	Workshop on System's Biology and Bioinformatics 2007	M. K Uni., Madurai	DBT & MKU
22.	Organizing Committee Member	Workshop on "Molecular Modelling and Pharmacoinformatics 2006	NIPER, Mohali.	DST & NIPER, Mohali
23.	Organizing Committee Member	Workshop on "Pharmacoinformatics in Drug Design 2005	NIPER, Mohali.	DST & NIPER, Mohali
24.	Organizing Committee Member	Workshop on Pharmacoinformatics: QSAR 2004	NIPER, Mohali.	DST & NIPER, Mohali

Events Participated (optional)

Conferences / Seminars / Workshops: 26

S. No.	Name of Conference	Place	Nature of presentation (Poster/Oral)
1.	International Conference on "Bioengineering Solutions for Healthcare, Food, Energy, and Environment" (BSHFEE 2021). (9th -10th April 2021)	IIT Jodhpur, Rajasthan	Attended
2.	19th International Conference on Bioinformatics (InCoB 2020), (25th – 29th Nov, 2020)	Virtually	Attended
3.	3rd International Conference on "Applied Nanoscience & Nanotechnology" (ICANN-2019). (18th – 19th March 2019)	Alagappa University, Karaikudi	Session Chaired

4.	International workshop on “Molecular Physiology, Therapeutics and Experimental Medicine (‘MPTEM’ 2016)”. (06th – 07th September, 2016)	Alagappa University, Karaikudi	Attended
5.	International conference on “Recent advances in modern medicine: Molecular signaling scenarios in tissues and diseases”. (03rd – 04th September, 2016)	SBMCH, Chennai	Attended
6.	6th International symposium on “Current Trends in Drug Discovery and Research” CTDDR - 2016	CSIR – CDRI, Lucknow	Attended
7.	Recent developments in Medical Biotechnology and Structure based Drug designing. (6th-7th December, 2015)	Indian Institute of technology, Guwahati	Chaired the session
8.	The 14th Theoretical chemistry Symposium, 2014	CSIR – National Chemical Laboratory, Pune	Attended
9.	Albany 2011: The 17th Conversation	University of Albany, New York, USA	Oral
10.	5th Annual Congress of International Drug Discovery Science and Technology Conference, 2007	Xian, China	Oral
11.	European Conference on Computation Biology - 2012	Swiss institute of Bioinformatics, University of Basel, Switzerland	Oral/Poster
12.	Current trends in Drug Discovery and Research- 2013	CSIR-Central Drug Research Institute, Lucknow, India	Oral
13.	Theoretical Chemistry Symposium (TCS-2012), 2012	Indian Institute of Technology, Guwahati, India	Oral
14.	Current Trends in Drug Discovery and Research- 2007	CSIR-Central Drug Research Institute, Lucknow, India	Oral
15.	International Conference on Bioinformatics (InCoB) 2006	New Delhi, India	Oral
16.	Indo-French Bioinformatics Meeting-2006	NCBS, Bangalore, India	Oral
17.	7th biannual discussion meeting in Theoretical chemistry, 2000	Indian Institute of Technology, Kanpur, India	Oral
18.	3rd National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design"	Alagappa University, Karaikudi	Oral
19.	Biotechmeet 2010	Madurai Kamaraj University, Madurai	Oral
20.	9th Tamil Science Conference, 2009	Alagappa University, Karaikudi	Oral
21.	4th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design, 2011	Alagappa University, Karaikudi	Oral
22.	5th International Symposium on Recent Trends in Macromolecular Structure and Function, 2012	University of Madras, Chennai	Oral

23.	Indo-US Workshop on Bio-computing, 2011	National Institute of Technology Calicut (NITC), India	Oral
24.	5th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design, 2012	Alagappa University, Karaikudi	Oral
25.	International Conference on Biomolecular Forms and Functions, 2013	Indian institute of science, Bangalore India	Oral
26.	Drug Development for Orphan/Neglected Diseases, 2013	CSIR- Central Drug Research Institute, Lucknow, India	Oral

Other Training Programs

- Teaching and Research in Bioinformatics and Chemo-informatics and related topics in **Centre of Excellence in Bioinformatics**, Madurai Kamaraj University, Madurai.
- Guest Faculty at **Dolphin Institute of Biomedical and Natural Sciences**, Deharadun for “Molecular Modeling and Bioinformatics”
- Taught theory and practical for M. Pharm. Students of Pharmacoinformatics at NIPER, Mohali.
- Conduct practical classes in a workshop of “**Pharmacoinformatics and Drug Design**” 14 -16 April at NIPER, Mohali.
- Conduct practical classes in “**Workshop of Molecular Modeling and Pharmacoinformatics**” 1-5 Nov. at NIPER, Mohali.
- Taken practical classes in **Workshop on Pharmacoinformatics: QSAR** 1-3 March 2006 at NIPER, Mohali.

Overseas Exposure / Visits

S. No	Country visited	Purpose of the Visit and place	Date and Year
1.	USA	Albany 2015: The 19th Conversation held at Department of Chemistry, University at Albany, New York	9 th to 13 th June, 2015
2.	Switzerland	European Conference on Computation Biology (ECCB-2012), A 11th European Conference on Computational Biology, held at the Swiss Institute of Bioinformatics, University of Basel.	9 th -12 th September, 2012
3.	Germany	European Molecular Biology Lab (EMBL), Heidelberg.	13 th September, 2012
4.	USA	Albany 2011: The 17th Conversation held at Department of Chemistry, University at Albany, New York.	14 th -18 th June, 2011.
5.	USA	Department of Chemistry and Structural Biology, and Computer Science lab at Stanford University, Stanford, California.	24 th -25 th June, 2011.
6.	China	Invited talk entitled “Quantitative structure activity relationship (3D-CoMFA Study) on Oxindole Derivatives as Cyclin Dependent Kinase 1 (CDK1) and Cyclin Dependent Kinase	7 th – 13 th November, 2007

		2 (CDK2) Inhibitors” in 5th Annual Congress of International Drug Discovery Science and Technology Conference’ (IDDSTTM), held at Xian.	
7.	China	Invited talk entitled “Drug Discovery Science and Technology Research” at Xian Technical University and Xian Technology Park.	7 th – 13 th November, 2007

Membership in

Professional Bodies

- Life Member of “Chemical Research Society of India (CRSI)”
- Life Member of “Protein Society (PS)” India
- Life Member of “Bioinformatics and Drug Discovery Society (BIDDS)”, India
- Life Member of “The Biotech Research Society(BRSI)” India
- Elected Life Member of “The National Academy of Sciences (NASI)” Allahabad, India
- Life Member of “Society for Biological Chemist (SBC)”
- Life Member of “Indian Biophysical Society (IBS)”
- Life Member of “The Indian Science Congress Association (ISCA)’.
- Life Member of ‘Society for Biotechnology (India)’.

Editorial Board

S. No	Position	Name of the journal and publisher	Period	
			From	To
1.		Edited a book on “ Innovations and Implementations of Drug Discovery Strategies in Rational Drug Design ” published by <i>Springer Nature in 2020</i> [ISBN 978-981-15-8936-2]		
2.	Editorial Board member	Journal of Microbiology and Biotechnology (JMB)	1 st January 2021	31 st December 2023
3.	Editorial Board member	Journal of AIDS and HIV Infection (JAH)	2017	Till date
4.	Editorial Board member	Journal of Microbiology and Biotechnology (JMB)	1 st April, 2016	31 st March, 2019
5.	Guest Editor	4 th issue entitled ‘Computer Aided Drug Design’ of BIOBYTES, Open Access Newsletter of Biotechnology Information System (BTIS) Department of Biotechnology (DBT), Government of India.		
6.	Guest Editor	Medicinal Chemistry, Bentham Science Publishers		
7.	Guest Editor	Special issue of SBCADD’2019 in the Journal of “Current Computer-Aided Drug Design” published by Bentham Science		

Academic Bodies (such as Board of Studies etc.,)

- Member of Board of Studies in Bioinformatics –UG/PG of Periyar University, Salem, 2016.
- **Chairman** of the University Rank Examination Question Paper Setting for M.Sc. Bioinformatics, Bharthidasan University, Trichy, Tamilnadu(2016).
- Member of Board of Central Evaluation in Bioinformatics, Pondicherry University in April 2009.
- External Member of programme Committee in Bioinformatics at Pondicherry University during Nov. 2010.
- Member Board of Studies of UGC Innovative programme on “Structural Pharmacogenomics”
- Member of Board of Studies of Bioinformatics, Alagappa University, Karaikudi from Nov 2010 to Nov, 2013.
- Member of board of Studies in Advance diploma in Molecular Modeling sponsored by DBT, New Delhi, Lady Dock College, Madurai Kamaraj University, Madurai.

Resource persons in various capacities

Number of Invited / Special Lectures delivered: 54

S. No.	Title of Lecture	Short Term Course/ Conference/Organization	Date	Organization
1.	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
2.	Advancement in computational Drug Discovery	E-learning program on Bioinformatics as Cartographic tool in Drug Discovery (Webinar)	May 21st, 2020	Dept. Of Bioinformatics, Alagappa University, Karaikudi
3.	Webinar cum hands on training	Computational Approaches for Anti-microbial Drug	21st August, 2020	Department of Biotechnology, Karpagam Academy of Higher Education
4.	Keynote Lecture	Emerging Trends in Biotechnological Advancements: Challenges and Prospects in Tackling Human Diseases	13th – 17th July, 2020	Department of Biotechnology, NIT, Warangal
5.	Keynote Lecture	Research Environment during the Post Covid Era” in the FDP-Webinar Series III	13th – 18th July, 2020	Holy Cross College, Tiruchirapalli, Tamil Nadu
6.	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	November 20-24, 2019	The Biotech Research Society, India
7.	Design of novel inhibitors to combat viral infection : A rational drug design approach	National Conference on Emerging Trends In Disease Model Systems -2019	March 25-27, 2019	NCCS, Pune

8.	Computational drug discovery approaches	Invited Lecture	January 23, 2019	Bishop Heber College, Trichy
9.	Molecular insights into the binding site for developing effective drugs	National Conference on Advanced Bio-Chem Development – 2018 (ABCD)	September 18-19, 2018	Sri Sarada Niketan College for Women, Karaikudi.
10.	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”	December 21, 2017	University of Hyderabad, Hyderabad
11.	Theoretical studies on HIV integrase inhibitors.	Invited Talk in National Conference on Innovations in Biotechnology (NCIB-2017)	December 14-15, 2017	Madurai Kamaraj University, Madurai
12.	<i>In silico</i> studies on HIV IN, Protease and Reverse Transcriptase.	International Conference on Innovations and Challenges in Biomedical Sciences Research	December 12-14, 2017	Holy Cross, Trichy
13.	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	3rd and 04, November 2017	Jamia Milia Islamia University, New Delhi
14.	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
15.	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
16.	Importance and Contribution of CADD and Molecular Modelling in HIV inhibitors	Occasion of Signing of MoUs	7 th March, 2016	Periyar University, Salem
17.	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
18.	Molecular Modeling and CADD in current Scenario	Remedial Coaching Class	22 nd January, 2016.	Alagappa University

19.	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
20.	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
21.	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
22.	Comprehensive Approach of Biotechnological Applications	Faculty Development Programme	16 th -29 th April, 2015	BIT, Anna University, Trichy.
23.	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
24.	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
25.	Theoretical Studies on HIV Integrase Inhibitors	Plenary lecture at National seminar on Bioinformatics (NSB'15)	28 th – 29 th January, 2015.	Bharathidasan University, Trichy.
26.	"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
27.	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
28.	Computer aided drug design and its importance in current drug discovery	National Conference on Bioengineering and Biotechnology An Industrial Perspective	16-17 Oct, 2014	AMITY, Lucknow

29.	Theoretical studies on CDK2 and HIV-Integrase inhibitors	National Conference on Society for Biotechnologies	November, 2013	S. G. B. Amravati University
30.	Currents trends in Pharmacoinformatics	Workshop on Molecular Modeling and Drug Design	14.07.2013 to 20.07.13	PSG college Coimbatore
31.	The molecular level energy calculation and Molecular dynamics studies on structurally similar HTLV and HIV protease enzymes using HIV-PR inhibitors	IWBIO-2013	18th -20th Mar, 2013	Granada, Spain
32.	A Theoretical Study of CDK2 Protein-Ligand Interactions through QM/MM interaction energy approach	Theoretical Chemistry Symposium	20.12.12	IIT, Ghawhati
33.	Molecular Docking of Small Molecules	National workshop on "Molecular Docking of Small Molecules"	27.01.11 to 29.01.11	Lady Dock College, Madurai
34.	CADD in Pharmaceutical Development	International year of chemistry Celebration	Oct, 2011	Gandhigram University, Dindigul
35.	Pharmacophoric study and QSAR model on Anti-Fungal Azoles	National Seminar on Advances in Bioinformatics	08.02.11	Holy Cross College, Trichy
36.	<i>In-Silico</i> screening in Drug Discovery	UGC sponsored academic staff college refresher course	03.12.10 to 18.12.10	Bhartidasan University, Trichy
37.	Ligand and Structure based Drug Design	UGC sponsored academic staff college refresher course	March, 2010	Amarawati University, Maharashtra
38.	Molecular Docking Studies on Antifungal Azoles	Genomics workshop	Nov. 2008	ILS Bhubaneswar
39.	Application of QSAR in Pharmaceutical Industry	CADD workshop	Oct. 2008	Pondicherry University
40.	CADD in pharmaceutical industry	Workshop on Industrial Bioinformatics	Feb. 2008	Bharathiyar University Coimbatore
41.	Over view of Molecular Modeling and Computer Aided Drug Design	Bioinformatics workshop	29.08.2007	JALMA Leprosy Institute (ICMR Lab), Agra
42.	"Computer Aided Drug Design"	Presentation in CTDDR	Feb. 07, 2007	CDRI Lucknow
43.	CADD and Bioinformatics	International Seminar on Bioinformatics	Nov. 2007	L. D. College, Madurai

44.	QPLD analysis on HIV-integrase inhibitors	National Workshop on "Recent trends in Bioinformatics"	11.09.2007 to 12.07.2007	School of Biotechnology, MKU, Madurai
45.	Pharmacophoric Studies on ACE inhibitors	Workshop on "Computer Aided Drug Design" in association with SCHRODINGER, USA.	6.03.2007 to 8.03.2007	School of Biotechnology, MKU, Madurai
46.	Challenges and Solution in CADD and Molecular Modeling	Silicon Graphics Technology Submit 2006	Dec. 2006	Chennai
47.	3D-QSAR CoMFA and CoMSIA study on Benzodipyrzoles as CDK2 Inhibitors	Workshop on Pharmaco-informatics: QSAR	01.03.06 to 03.03.06	NIPER, Mohali, India
48.	QSAR studies on indenopyrazole derivatives	Indo-French Bioinformatics Meeting	12.06.06 to 14.06.06	NCBS, Bangalore
49.	Virtual screening on CDK inhibitors	Workshop on Systems Biology and its application	6.09.2006 to 8.09.2006	School of Biotechnology, MKU, Madurai
50.	3D-QSAR studies on benzodipyrzole series of CDK inhibitors	National Workshop on "Pharmaco-informatics in Drug Design"	14-16 April 2005	(NIPER) Mohali, Punjab.
51.	QSAR studies on indenopyrazole derivatives	9th biannual discussion meeting in theoretical Chemistry	9-12 Dec 2005	BARC, Mumbai
52.	Quantum Pharmacological study on HIV-1RT Inhibitors	7th biannual discussion meeting on Theoretical Chemistry	Jan. 2004	IIT Kanpur
53.	QSAR studies on indenopyrazole derivatives	9th biannual discussion meeting in Theoretical Chemistry	09.12.04 to 12.12.04	BARC, Mumbai
54.	Pharmacophoric features of HIV-1RT inhibitors	8th biannual discussion meeting in Theoretical Chemistry	17.01.03 to 19.01.03	IACS, Jhadavpur, Kolkata

Others

1. Articles published in Newspapers / Magazines : 02
2. No. of PhD Thesis evaluated : 35
3. No. of PhD Public Viva Voce Examination conducted : 26
4. Sequences submitted in
 - Gene Sequence : 7627
 - Protein Sequence : 7627
 - 16S rRNA gene sequence : 4
 - Genome sequence : 2
 - NGS data submitted to SRA, NCBI database
 - DNA-seq : 2
 - Biosample : 2

Publications

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1. Velmurugan, k., Derin, D., Kannan, R., Selvaraj, C., Vishnupriya, S., Selvaraj, G., **Singh, S.K.**, Nandhakumar, R., Synthesis, antibacterial, anti-oxidant and molecular docking studies of imidazoquinolines. *Cell Press-Heliyon* 2021, p.e07484 (IF-0.0).
2. Chandra, I., Prabhu, S.V., Nayak, C., **Singh, S.K***, E-pharmacophore based screening to identify potential HIV-1 gp120 and CD4 interaction blockers for wild and mutant types. *SAR and QSAR in Environmental Research* 2021, 32(5), pp.353-377 (IF-3.00).
3. Aarthy, M., **Singh, S.K***, Interpretations on the Interaction between Protein Tyrosine Phosphatase and E7 Oncoproteins of High and Low-Risk HPV: A Computational Perception. *ACS Omega* 2021, 6(25), pp.16472–16487 (IF-3.51).
4. Selvaraj, C., Dinesh, DC., Krafcikova, P., Boura, E., Aarthy, M., Pravin, MA., **Singh, S.K***, Structural Understanding of SARS-CoV-2 Drug Targets, Active Site Contour Map Analysis and COVID-19 Therapeutics. *Current Molecular Pharmacology* 2021 (Accepted) (IF-3.33).
5. Kalamurthi, S., Selvaraj, G., Selvaraj, C., **Singh, S.K.**, Wei, D. Q., Peshherbe, G. H., Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. *International Journal of Molecular Sciences* 2021, 22(13), pp.7071 (IF-5.92).
6. Panwar, U., **Singh, S.K***, *In silico* virtual screening of potent inhibitor to hamper the interaction between HIV-1 integrase and LEDGF/p75 interaction using E-pharmacophore modeling, molecular docking, and dynamics simulations. *Computational Biology and Chemistry* 2021, p.107509 (IF-2.87).
7. Dwivedi, A., Kumari, A., Aarthy, M., **Singh, S.K.**, Ojha, M., Jha, S., Jha, S.K., Jha, N.S., Spectroscopic and molecular docking studies for the binding and interaction aspects of curcumin-cysteine conjugate and rosmarinic acid with human telomeric G-quadruplex DNA. *International Journal of Biological Macromolecules* 2021, 182, pp.1463 – 1472 (IF-6.95).
8. Selvaraj C., Selvaraj G., Ismail RM., Baazeem A., Wei DQ., **Singh, S.K***, Interrogation of Bacillus anthracis SrtA active site loop forming open/close lid conformations through extensive MD simulations for understanding binding selectivity of SrtA inhibitors. *Saudi Journal of Biological Sciences* 2021, 28(7), pp.3650-3659 (IF-4.21).
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10. Qureshi, S., Khandelwal, R., Madhavi, M., Khurana, N., Gupta, N., Choudhary, S.K., Suresh, R.A., Hazarika, L., Srija, C.D., Sharma, K., Hindala, M.R., Hussain, T., Nayariseri, A., **Singh, S.K***, A Multi-Target Drug Designing for BTK, MMP9, Proteasome and TAK1 for the

clinical treatment of Mantle Cell Lymphoma. *Current Topics in Medicinal Chemistry* 2021, 21(9), pp.790-818 (IF-3.29).

11. Nayariseri, A., Khandelwal, R., Tanwar, P., Madhavi, M., Sharma, D., Thakur, G., Speck-Planche, A., **Singh, S.K***, Artificial Intelligence, Big data and Machine Learning approaches in Precision Medicine & Drug Discovery. *Current drug targets* 2021, 22(6), pp.631-655 (IF-3.46).

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12. Selvaraj, C., Panwar, U., Dinesh, DC., Bouřa, E., Sing, P., Dubey, V.K., **Singh, S.K***, Microsecond MD Simulation and Multiple-Confirmation Virtual Screening to Identify Potential Anti-COVID-19 Inhibitors Against SARS-CoV-2 Main Protease. *Frontiers in Chemistry* 2020, 8, p.1179 (IF-5.22).
13. Selvaraj, C., Dinesh, DC., Panwar, U., Bouřa, E., **Singh, S.K***, High-Throughput Screening and Quantum Mechanics for Identifying Potent Inhibitors against Mac1 Domain of SARS-CoV-2 Nsp3. *IEEE/ACM Transactions on Computational Biology and Bioinformatics* 2020, DOI:10.1109/TCBB.2020.3037136 (IF-3.71).
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22. Panwar, U., **Singh, S. K***, Atom-based 3D-QSAR, molecular docking, DFT, and simulation studies of acylhydrazone, hydrazine, and diazene derivatives as IN-LEDGF/p75 inhibitors. *Structural Chemistry* 2020, pp.1-16 (IF-1.88).
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Reviewer of Journals

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Bioorganic and Medicinal Chemistry Letters	FEMS Microbiology Letters
Bioorganic and Medicinal Chemistry	RSC Advances

Pattern Recognition Letters	Molecular Biosystems
Plos Computational Biology	Chemical Biology and Drug Design
Proteins: Structure, Function and Bioinformatics	Plos one
Journal of Biomolecular Structure and Dynamics	Journal of Molecular Graphics and Modelling
SAR and QSAR in Environmental Research	Microbial Pathogenesis
Medicinal Chemistry	Molecular Simulations
Current Computer-Aided Drug Design	Journal of Proteins and Proteomics
Medicinal Chemistry Research	Journal of Molecular Recognition
Journal of Theoretical Biology	Journal of Receptor and Signal Transduction
Journal of Molecular Structure	Journal of Enzyme inhibition and Medicinal Chemistry
Journal of Pesticide Biochemistry and Physiology	Current Pharmaceutical Design
ACS Chemical Neuroscience	ACS Omega
ACS Medicinal Chemistry Letters	ACS Combinatorial Science
Nature Scientific Reports	ACS Journal of Physical Chemistry Letters
Microbiology & Biotechnology Letters	Computers in Biology & Medicine
Pesticide Biochemistry & Physiology	International Journal of Biological Macromolecules
Biomed Research International	Proteins and Peptide letters
Progress in Biophysics and Molecular Biology	Expert Opinion in Drug Discovery
Drug Discovery Today	BBA Proteins and Proteomics