Dr. Sanjeev Kumar Singh
Professor

Contact

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Academic Qualifications: M.A./M.Sc./M. Phil. /Ph.D. /

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: 17 Years

Research Experience: 17 Years

Designation	Name of Employer	Period		No. of Years /Months
		From	To	
Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	20th March, 2015	**Continue**	**2 years & 5 months**
Associate Professor	Dept. of Bioinformatics Alagappa University Karaikudi, Tamil Nadu	20th March, 2012	19th March, 2015	3 years
Reader	Dept. of Bioinformatics Alagappa University Karaikudi	20th March, 2009	19th March, 2012	3 years
Lecturer	CoE in Bioinformatics, School of Biotechnology, Madurai Kamaraj University	31st March, 2006	19th March, 2009	3 years
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 Community Services**
  - Involved in the activity of "**Village Placement program**" conducted by Alagappa University.
  - **Nodal Officer** for the "**Ek Bharat Shreshta Bharat**" Scheme under the Ministry of Human Resource and Development (Govt. of India) from Alagappa University.

- **Responsibility in Corporate Life**
  - Invited for lecture and training in personality development at Department of Bank Management, Alagappa University, karaikudi.
  - Invited for lecture and training in personality development at Bharthidasan University, Trichy.

- **Nominated as the inspection team member for affiliation DDE Centre's:**
  - Kurinji College of Arts and Science, Gateway for Entrepreneurship and Management Studies Trust, Trichy.
  - Dharmapuram Adhinam Arts College, Sree Radhaa Krishna Educational Trust, Mayiladuthurai.

Areas of Research

Our aims to improve treatment and develop novel therapeutics from basic research to molecular level for the study of interactive small chemical inhibitors with biological targets such as Cyclin-dependent kinases (CDKs), Human immunodeficiency virus (HIV), Histone Acetyltransferase (HAT), Human G Protein-coupled Receptor (h-GPCR), Retinoblastoma/HPV and to portray their mechanism towards the novel discovery. We explore and design pharmacologically relevant ligand that can act as specific and potent inhibitors of various target activity on the premise of combined *in-silico* approaches, including Molecular Modelling, Biophysical methods, Structural Bioinformatics and Computational Biology. 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 calculation, Free energy calculation, Pharmacophore mapping and Quantum Polarized Ligand docking (QPLD). In order to develop new models, Ab initio Quantum calculation, 3D-database searching & development, combinatorial library design, Optimization of lead compounds and Molecular Dynamics simulations are used to contribute in drug designing and discovery process.Our energetic environment of team work is focused to gain the experience and knowledge for developing research strategies to support the current scenario of drug discovery.

Research Supervision / Guidance

Program of Study		Completed	Ongoing
Research	**Ph.D.**	03	07
	Post Doc	01	-
	M.Phil.	08	-
Project	**PG**	26	-
	UG / Others	06	-

Publications

International Journals	National Journals	Book Chaptesrs
76	**06**	**12**

Cumulative Impact Factor (as per JCR) : 164.216
h-index : 13
i10 index : 20
Total Citations : 522

Funded Research Projects

Completed Projects

S. No	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
1	CSIR, New Delhi	2012	2015	QM/MM partial charges, binding pocket contours analysis and FEP calculation for designing potent inhibitors of HTLV- Protease: A *De novo* drug design approach	**16.02**
2	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**
3	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**
4	AURF (UGC) with NIBI, Osaka	2009	2012	Pharmacophoric Analysis and designing of ATP competitive CDK 4 inhibitors.	**4.00**

Ongoing Projects

S. No.	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
1	DBT New Delhi	2016	2019	*In-Silico* screening, theoretical calculation and in vitro studies for development of potential HIV1-PR inhibitors	**19.51**
2	DBT-Twin Project with IIT, Guwahati	2014	2017	Identification of novel drug targets of *Leishmania donovani*: Studies on CAAX prenyl protease I and II of the pathogen	**73.69**

PROJECTS IN REVIEW PROCESS

S. NO.	Project Title	Funding Agency	Budget (Rs. In lakhs)	In Process
1	National Drug Discovery against Zika Virus.	DST-BRICS, New Delhi	**40.00**	Under review process
2	Exploration on the stability and interactions of the Retinoblastoma in association with the HPV and CDK through in silico and in vitro analysis	DST SERB,	**52.47**	Under review process
3	An integrated in silico and in vitro approaches for Potential selective inhibitors of PCAF as epigenetic target for cancer therapy	DBT New Delhi	**142.00**	Under review process

Patents

- **Nil**

Distinctive Achievements / Awards

- **Special Officer (Liaison with Funding Agencies)** at Alagappa University (Sep, 2017).
- **Deputy Coordinator**, DST-FIST Program (Level-I) (2017).
- **ICMR Lala Ram Chand Kandhari Award** for his outstanding contribution in research works on Sexually Transmitted Diseases, entitled "*In silico* studies on HIV-1 Integrase and Protease to find potent inhibitors". (2016)
- **Liaison Officer** at Alagappa University (From 16 Sep, 2016 to 15 Sep, 2017).
- **Department Coordinator** of UGC-NAAC at Department of Bioinformatics, Alagappa University (2016).
- Council for Scientific and Industrial Research (CSIR) Travel Award: To present paper in **"Albany 2015: The 19th Conversation"** held at Department of Chemistry, University at Albany, New York, USA
- Indian Council of Medical Research (ICMR) Travel Award: To present paper in **ECCB-12** at Basel, Switzerland (2012).
- Department of Science and Technology (DST) Travel Award: To present paper in **"Albany 2011: 17th Conversation"** at University of Albany, USA (2011).
- **DST Fast Track grant** for Young Scientist-2010 in Chemical Science.
- Department of Biotechnology (DBT) Travel Award: To present a paper in IDDST-2007 in Xian, China (2007).

Achievements by Students

- **Sunil Kumar Tripathi,**(Student) CSIR-SRF Award -2012 in Bioinformatics
- **Chandrabose Selvaraj** (Student) Asia Pacific Bionetwork and Bioclues Travel Award-2012 to work in A-Star institute at Singapore for one month.
- **Chandrabose Selvaraj** (Student) BIRD -Special Mention Award-2012.
- **Venkatesan Suryanarayanan** (Student) DST-Inspire Fellowship Award – 2012.
- **Karnati Konda Reddy** (Student) CSIR –SRF Award -2013 in Bioinformatics.
- **KK Reddy** ICMR travel grant to present paper in ISMB/ECCB conference in Berlin, Germany, 2013.
- **Umesh Panwar** (Student) Alagappa University Fellowship (AURF - 2015-2017).
- **Aarthy M**. (Student) Rajiv Gandhi National Fellowship (RGNF) - UGC -(2015-2017).

Events organized in leading roles

Number of Seminars / Conferences / Workshops / Events organized: 17

S. No	Designation	Title	Organized at	Sponsors
1	Organizing Secretary	9th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2017	Alagappa University, Karaikudi	ICMR, TNSTC & Alagappa University
2	Organizing Secretary	9th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2014	Alagappa University, Karaikudi	ICMR & Alagappa University
3	Organizing Committee Member	International Conference on Recent Trends in Biosciences (ICRTB) April, 2016	Alagappa University, Karaikudi	Alagappa University
4	Organizing Committee Member	8th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2016	Alagappa University, Karaikudi	DBT & Alagappa University
5	Organizing Committee Member	7th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2015	Alagappa University, Karaikudi	DBT, DST, & CSIR
6	Organizing Secretary	6th National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" 2014	Alagappa University, Karaikudi	DBT & Alagappa University
7	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
8	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
9	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
10	Convener	2nd National Workshop on "Application of Molecular Modeling and Structural Bioinformatics" 2010	Alagappa University, Karaikudi	DBT & Alagappa University
11	Organizing	Workshop on "Computer Aided Drug Design" 2009	M. K Uni.,	DBT &

	Secretary		Madurai	MKU
12	Organizing Secretary	Workshop on Systems Biology and its application 2008	M. K Uni., Madurai	DBT & MKU
13	Organizing Secretary	Workshop on Bioinformatics Software's 2008	M. K Uni., Madurai	DBT & MKU
14	Organizing Secretary	Workshop on System's Biology and Bioinformatics 2007	M. K Uni., Madurai	DBT & MKU
15	Organizing Committee Member	Workshop on "Molecular Modelling and Pharmacoinformatics 2006	NIPER, Mohali.	DST & NIPER, Mohali
16	Organizing Committee Member	Workshop on "Pharmacoinformatics in Drug Design 2005	NIPER, Mohali.	DST & NIPER, Mohali
17	Organizing Committee Member	Workshop on Pharmacoinformatics: QSAR 2004	NIPER, Mohali.	DST & NIPER, Mohali

Events Participated (optional)

Conferences / Seminars / Workshops: 23

S. No.	Name of Conference	Place	Nature of presentation (Poster/Oral)
1	International workshop on "Molecular Physiology, Therapeutics and Experimental Medicine ('MPTEM' 2016)". (06^{th} – 07^{th} September, 2016)	Alagappa University, Karaikudi	Attended
2	International conference on "Recent advances in modern medicine: Molecular signaling scenarios in tissues and diseases". (03^{rd} – 04^{th} September, 2016)	SBMCH, Chennai	Attended
3	6^{th} International symposium on "Current Trends in Drug Discovery and Research" CTDDR - 2016	CSIR – CDRI, Lucknow	Attended
4	Recent developments in Medical Biotechnology and Structure based Drug designing. (6^{th}-7^{th} December, 2015)	Indian Institute of technology, Guwahati	Chaired the session
5	The 14^{th} Theoretical chemistry Symposium, 2014	CSIR – National Chemical Laboratory, Pune	Attended
6	Albany 2011: The 17th Conversation	University of Albany, New	Oral

		York, USA	
7	5th Annual Congress of International Drug Discovery Science and Technology Conference, 2007	Xian, China	Oral
8	European Conference on Computation Biology - 2012	Swiss institute of Bioinformatics, University of Basel, Switzerland	Oral/Poster
9	Current trends in Drug Discovery and Research-2013	CSIR-Central Drug Research Institute, Lucknow, India	Oral
10	Theoretical Chemistry Symposium (TCS-2012), 2012	Indian Institute of Technology, Guwahati, India	Oral
11	Current Trends in Drug Discovery and Research-2007	CSIR-Central Drug Research Institute, Lucknow, India	Oral
12	International Conference on Bioinformatics (InCoB) 2006	New Delhi, India	Oral
13	Indo-French Bioinformatics Meeting-2006	NCBS, Bangalore, India	Oral
14	7th biannual discussion meeting in Theoretical chemistry, 2000	Indian Institute of Technology, Kanpur, India	Oral
15	3rd National Symposium cum Workshop on "Recent Trends in Structural Bioinformatics And Computer Aided Drug Design"	Alagappa University, Karaikudi	Oral
16	Biotechmeet 2010	Madurai Kamaraj University, Madurai	Oral
17	9th Tamil Science Conference, 2009	Alagappa University, Karaikudi	Oral
18	4th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design, 2011	Alagappa University, Karaikudi	Oral
19	5th International Symposium on Recent Trends in Macromolecular Structure and Function, 2012	University of Madras, Chennai	Oral
20	Indo-US Workshop on Bio-computing, 2011	National Institute of Technology Calicut (NITC), India	Oral
21	5th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design, 2012	Alagappa University, Karaikudi	Oral
22	International Conference on Biomolecular Forms and Functions, 2013	Indian institute of science, Bangalore India	Oral

23	Drug Development for Orphan/Neglected Diseases, 2013	CSIR- Central Drug Research Institute, Lucknow, India	Oral

Resource persons in various capacities

Number of Invited / Special Lectures delivered: 41

S. No.	Title of Lecture	Short Term Course/ Conference/Organization	Date	Organization
1.	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
2.	Computers in Drug Discovery	Invited for delivering a plenary lecture at Department of Information Technology	24th August, 2016	Dr. Umayal Ramanathan College for Women, Karaikudi
3.	Importance and Contribution of CADD and Molecular Modelling in HIV inhibitors	Occasion of Signing of MoUs	7th March, 2016	Periyar University, Salem
4.	Theoretical studies on HIV-1 Integrase Inhibition by Strand Transfer and LEDGF/P75 Binding site Inhibitors	Annual meeting of the Indian Biophysical Society	9th February, 2016	Indian Biophysical Society, Bangalore
5.	Molecular Modeling and CADD in current Scenario	Remedial Coaching Class	22nd January, 2016.	Alagappa University
6.	Impact of Computer aided drug design and Molecular modeling in current drug discovery	Recent developments in Medical Biotechnology and Structure based Drug designing	6th-7th December, 2015	Indian Institute of technology, Guwahati
7.	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	7th December, 2015	Indian Institute of technology, Guwahati
8.	Molecular Modeling and Dynamics Studies of HIV & HTLV Inhibitors	Symposium cum Workshop on "Advances in Computational Biology and Computer Aided Drug Design" during	24th-26th, June, 2015	BSBE, Indian Institute of Technology Guwahati
9.	Comprehensive Approach of Biotechnological	Faculty Development Programme	16th -29th April, 2015	BIT, Anna University,

	Applications			Trichy.
10.	Current Topics in CADD	Key note address at National seminar on Genomics and Proteomics: A Computational Approach	6th March, 2015.	Lady Dock College, Madurai
11	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)	5th March, 2015	Periyar University, Salem
12	Theoretical Studies on HIV Integrase Inhibitors	Plenary lecture at National seminar on Bioinformatics (NSB'15)	28th – 29th January, 2015.	Bharathidasan University, Trichy.
13.	"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"	3rdMarch, 2015.	MaduariKamaraj University, Madurai on
14.	QM/MM studies on HIV-Integrase Strand Transfer Inhibitors	Recent Strategies in Drug Discovery - III	25th - 27th, September 2014	PSG college of Arts and Science, Coimbatore
15.	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
16.	Theoretical studies on CDK2 and HIV-Integrase inhibitors	National Conference on Society for Biotechnologies	November, 2013	S. G. B. Amravati University
17.	Currents trends in Pharmacoinformatics	Workshop on Molecular Modeling and Drug Design	14.07.2013 to 20.07.13	PSG college Coimbatore
18.	The molecular level energy calculation and Molecular dynamics studies on structurally similar HTLV and HIV protease enzymes using HIV-PR inhibitors	IWBBIO-2013	18th -20th Mar, 2013	Granada, Spain
19.	A Theoretical Study of CDK2 Protein-Ligand Interactions through QM/MM interaction energy approach	Theoretical Chemistry Symposium	20.12.12	IIT, Ghawhati
20.	Molecular Docking of Small Molecules	National workshop on "Molecular Docking of Small Molecules	27.01.11 to 29.01.11	Lady Dock College, Madurai

21.	CADD in Pharmaceutical Development	International year of chemistry Celebration	Oct, 2011	Gandhigram University, Dindigul
22.	Pharmacophoric study and QSAR model on Anti-Fungal Azoles	National Seminar on Advances in Bioinformatics	08.02.11	Holy Cross College, Trichy
23.	*In- Silico* screening in Drug Discovery	UGC sponsored academic staff college refresher course	03.12.10 to 18.12.10	Bhartidasan University, Trichy
24.	Ligand and Structure based Drug Design	UGC sponsored academic staff college refresher course	March, 2010	Amarawati University, Maharashtra
25.	Molecular Docking Studies on Antifungal Azoles	Genomics workshop	Nov. 2008	ILS Bhubaneswar
26.	Application of QSAR in Pharmaceutical Industry	CADD workshop	Oct. 2008	Pondicherry University
27.	CADD in pharmaceutical industry	Workshop on Industrial Bioinformatics	Feb. 2008	Bharathiyar University Coimbatore
28.	Over view of Molecular Modeling and Computer Aided Drug Design	Bioinformatics workshop	29.08.2007	JALMA Leprosy Institute (ICMR Lab), Agra
29.	"Computer Aided Drug Design"	Presentation in CTDDR	Feb. 07, 2007	CDRI Lucknow
30.	CADD and Bioinformatics	International Seminar on Bioinformatics	Nov. 2007	L. D. College, Madurai
31.	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
32.	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
33.	Challenges and Solution in CADD and Molecular Modeling	Silicon Graphics Technology Submit 2006	Dec. 2006	Chennai
34.	3D-QSAR CoMFA and CoMSIA study on Benzodipyrazoles as CDK2 Inhibitors	Workshop on Pharmacoinformatics: QSAR	01.03.06 to 03.03.06	NIPER, Mohali, India
35.	QSAR studies on indenopyrazole derivatives	Indo-French Bioinformatics Meeting	12.06.06 to 14.06.06	NCBS, Bangalore

36.	Virtual screening on CDK inhibitors	Workshop on Systems Biology and its application	6.09.2006 to 8.09.2006	School of Biotechnology, MKU, Madurai
37.	3D-QSAR studies on benzodipyrazole series of CDK inhibitors	National Workshop on "Pharmacoinformatics in Drug Design"	14-16 April 2005	(NIPER) Mohali, Punjab.
38.	QSAR studies on indenopyrazole derivatives	9th biannual discussion meeting in theoretical Chemistry	9-12 Dec 2005	BARC, Mumbai
39.	Quantum Pharmacological study on HIV-1RT Inhibitors	7th biannual discussion meeting on Theoretical Chemistry	Jan. 2004	IIT Kanpur
40.	QSAR studies on indenopyrazole derivatives	9th biannual discussion meeting in Theoretical Chemistry	09.12.04 to 12.12.04	BARC, Mumbai
41.	Pharmacophoric features of HIV-1RT inhibitors	8th biannual discussion meeting in Theoretical Chemistry	17.01.03 to 19.01.03	IACS, Jhadavpur, Kolkata

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

- **Albany** 2015, The 19th Conversation held at Department of Chemistry, University at Albany, New York, USA during 9th to 13th, June, 2015.
- **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, Switzerland, during 9-12 September, 2012.

- **Germany:** European Molecular Biology Lab (EMBL), Heidelberg, Germany, 13th September, 2012.
- **USA:** Albany 2011, The 17th Conversation held at Department of Chemistry, University at Albany, New York, USA during 14-18 June, 2011.
- **USA:** Department of Chemistry and Structural Biology, and Computer Science lab at Stanford University, Stanford, California, during 24-25 June, 2011.
- **China:** Invited talk entitled "Quantitative structure activity relationship (3D-CoMFA Study) on Oxindole Derivatives as Cyclin Dependent Kinase 1 (CDK1) and Cyclin Dependent Kinase 2 (CDK2) Inhibitors" in 5th Annual Congress of International Drug Discovery Science and Technology Conference' (IDDSTTM), held at Xian, China during 7- 13th November, 2007.
- **China:** Invited talk entitled "Drug Discovery Science and Technology Research" at Xian Technical University and Xian Technology Park, China, 2007

Membership in

Professional Bodies

- Life Member of "The Biotech Research Society(BRSI)"
- Life Member of "The National Academy of Sciences (NASI)"
- 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

- **Editorial Board member** of **Jounral of AIDS and HIV Infection (JAHI).**
- **Editorial board member of Journal of Microbiology and Biotechnology (JMB)** for the period of 1st April, 2016 to 31st March, 2019 (3 years)
- **Department Coordinator of UGC-NAAC** at Department of Bioinformatics, Alagappa University (2016).
- **Guest Editor** of 4th issue entitled 'Computer Aided Drug Design' of BIOBYTES, Open Access Newsletter of Biotechnology Information System (BTIS), Department of Biotechnology (DBT), Government of India.
- **Guest Editor**, **Medicinal Chemistry**, Bentham Science Publishers.
- Special Invitee in Senate of Alagappa University in 2009.
- Special Invitee in Syndicate meeting of Academic Affairs in Alagappa University at Karaikudi.

Advisory Board

- Member of 'Trends on Theoretical Chemistry' Biannual Conference.
- Member of 'Indo-French Bioinformatics Meeting'.

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.

Others

1. Articles published in Newspapers / Magazines : 02
2. No. of PhD Thesis evaluated : 20
3. No. of PhD Public Viva Voce Examination conducted : 15
4. Sequences submitted in GenBank: 04

Recent Publications

PUBLICATIONS

2017

1. Sharda S, Sarmandal P, Cherukommu S, Dindhoria K, Yadav M, Bandaru S, Sharma A, Sakhi A, Vyas T, Hussain T, Nayarisseri A, **Singh SK** .A Virtual Screening approach for the Identificationof High affinity small molecules targeting BCR-ABL1 inhibitors for the treatment of Chronic Myeloid Leukemia. ***Curr Top Med Chem***. 2017; DOI: 10.2174/1568026617666170821124512, **[Accepted] (IF: 2.561).**
2. Natesan K, Arumugasamy K, Thangaraj K, Antony S, Vaiyapuria M, **Singh SK** , Cyril R, Lee SM. Elucidation on effect of Pelargonidin towards cell cycle regulators and DNA methyltransferases in human colorectal cancer cells: A molecular dynamic simulation approach. ***Comput Biol Chem***. 2017**; [Accepted] (IF: 1.331).**

3. Sharma N, Aarthy M, Singh SK, Giri R. Epigallocatechin gallate, an active green tea compound inhibits the Zika virus entry into host cells via binding the envelope protein. ***Int J Biol Macromol.*** 2017; **[Accepted] (IF: 3.671).**

4. Thangaraj K, Arumugasamy K, Natesan K, Ramasamy S, Cyril R, **Singh SKS** and Vaiyapuri M. *In Silico* Molecular Docking Analysis Of Orientin, A Potent Glycoside of Luteolin against BCL-2 Family Proteins. ***J chem pharm res.*** 2017; 9(5):65-72 **(IF:0.64).**

5. Srinivas B, Sumithnath T.G, Sharda S, Lakhotia S, Sharma A, Hussain T, Jain A, Nayarisseri A, **Singh S.K**. Helix-coil transition signatures BRAF V600E mutation and virtual screening for inhibitors directed against mutant BRAF. ***Curr Drug Metab.*** 2017;]DOI: 10.2174/1389200218666170503114611 **[Accepted]** (**IF: 2.659**).

6. Nivedha RP, Suryanarayanan V, Selvaraj C, **Singh SK**, Rajalakshmi M. Chemopreventive effect of saponin isolated from Gymnema sylevestre on prostate cancer through in silico and in vivo analysis. ***Med Chem Res.*** 2017**;** DOI: 10.1007/s00044-017-1900-3 **[Accepted]** (**IF: 1.277**).

7. Bhardwaj R , Das M , Singh S, Chiranjivi AK, Prabhu SV, **Singh SK**, Dubey VK . Evaluation of CAAX prenyl protease II of *Leishmania donovani* as potential drug target: infectivity and growth of the parasite is significantly lowered after the gene knockout. ***Eur J Pharm Sci.*** 2017**;** 102:156–160 **(IF: 3.756).**

8. Gupta S, Suryanarayan V, Yadav S, **Singh SK**, Saxena JK. Delineating the role of ionic interactions in structural and functional integrity of B. malayi Guanylate kinase. ***Int J Biol Macromol.*** **2017;** 98:357-365 **(IF: 3.671).**

9. Prabhu SV, Tiwari K, Suryanarayanan V, Dubey VK, **Singh SK.** Exploration of new and potent lead molecules against CAAX prenyl protease I of Leishmania donovani through Pharmacophore based virtual screening approach. ***Comb Chem High Throughput Screen.*** 2017; [**Accepted**] **(IF-0.952)**.

10. Aarthy M, Panwar U, Selvaraj C**, Singh SK**. Advantages of Structure-Based Drug Design Approaches in Neurological Disorders. ***Curr Neuropharmacol.*** 2017**;** DOI: 10.2174/1570159X15666170102145257 **(IF-3.365)**.

11. Gupta S, Yadav S, Suryanarayanan V, **Singh SK**, Saxena JK. Investigating the folding pathway and substrate induced conformational changes in B. malayi Guanylate kinase. ***Int J Biol Macromol.*** 2017; 94(Pt A):621-633 **(IF-3.671).**

2016

12. Selvaraj C, Krishnasamy G, Jagtap S.S, Patel S.K.S, Dhiman S.S, Kim Tae-Su, **Singh SK**, Lee J.K. Structural insights into the binding mode of d-sorbitol with sorbitol dehydrogenase using QM-polarized ligand docking and molecular dynamics simulations. ***Biochem Eng J.*** 2016**;** 114: 244-256 **(IF-2.892).**

13. Sivakamavalli J, Selvaraj C, **Singh SK,** Vaseeharan B. Modelling of macromolecular proteins in prophenoloxidase cascade through experimental and computational approaches. ***Biotechnol Appl Biochem.*** **2016; 63(6):779-788(IF=1.413).**

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- Experience in designing novel chemical entities for various therapeutic areas and calculating interaction energies of the molecules within active site residues of biological targets.
- Experience of using Windows, LINUX, UNIX and Mac operating system.
- Experienced in using other Molecular Modeling, Computational Chemistry and Bioinformatics software's like , SYBYL 7.0, Discovery Studio, CCDC, GOLD, MOE, Cerius2, Insight II, TOPKAT, CHEM-X, Bio Suite, GCG, SCHRODINGER Software, AMBER, GROMACS, Marvin Suit, Modeller, AUTODOCK etc.
- Experience of various M.O. Calculations packages like GAUSSIAN 03 (Linux & windows), SPARTAN
- Experienced in using visualization software like PyMol, PDB Viewer, Rasmol, NOC, MOLDEN, MOLEKEL, Chimera, VMD etc.
- Working experience on Centos workstation, SUN workstation, SGI- Altix (6 CPUs), SGI-Tezro (4 CPUs), SGI Power Onyx, Octane 2, SGI Fuel, IBM server and HP multi processor cluster.
- Knowledge of biological databases and development.
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