

# Curriculum Vitae

Gajendra P. S. Raghava

## PERSONAL DETAILS

Name: **Gajendra P. S. Raghava**

Current Position: **Professor**

Date of Birth: **25<sup>th</sup> May 1963**

Organization/Institute: **IIIT, Delhi**

Web Site <http://webs.iiitd.edu.in/raghava/>

Google Scholar: [XK5GUiYAAAAJ](#)

Email: **ragahva@iiitd.ac.in**

## EDUCATION QUALIFICATION & EXPERIENCE

### Academic Qualification (Bachelor's Degree onwards)

Degree	Institution	Year	Percentage
Ph. D.	IMTECH/Panjab Univ. Chandigarh	1996	N/A
M. Tech.	Indian Institute of Technology, Delhi	1986	7.41 CGPA
M. Sc.	Meerut University, Meerut	1984	68.9%
B. Sc.	Meerut University, Meerut	1982	66.4%

### Positions held in chronological order

Period		Place of Employment	Designation	Scale of Pay
From	To			
1986	1991	IMTECH, Chandigarh	Scientist-B	Rs 700-1400
1991	1996	----- do -----	Scientist-C	Rs 3000-4500
1996	2002	----- do -----	Scientist-E1	Rs 12000-16000
2002	2007	----- do -----	Scientist-EII	PBIV GP 8700
2008	2013	----- do -----	Scientist-F	PB IV GP 8900
2013	2017	----- do -----	Chief Scientist	PB IV GP 10000
2017	2020	IIIT, Delhi	Professor	PB IV GP 10500
2020	Cont.	IIIT, Delhi	Professor (HAG)	HAG Scale (Level 15)

### Significant foreign assignments

Period of visit		Institute/ country visited	Purpose of visit
From	To		
August 1996	July 1998	Oxford University, Oxford, UK	Worked as Post-Doctoral fellow
Sept. 2002	March 2003	UAMS, Little Rock, USA	To establish bioinformatics infrastructure at UAMS
March 2004	August 2004	POSTECH, South Korea	Worked as visiting professor
March 2006	Sept. 2006	UAMS, Little Rock, USA	Advanced infrastructure for research in bioinformatics.

## HONORS & AWARDS

➤ **Fellow of National Academies**

1. Fellow of National Academy of Sciences (FNASc.), India
2. Fellow of Indian Academy of Sciences (FASc.), Bangalore
3. Fellow of Indian National Science Academy (FNA), Delhi

➤ **Major National Awards/recognitions**

1. National Bioscience Award for Career Development 2006, by DBT
2. Shanti Swarup Bhatnagar Award 2008 in Biological Sciences
3. NASI-Reliance Industries Platinum Jubilee Award (2009)
4. JC Bose National Fellowship, 2010-15 & 2015-2020 by DST, India
5. Lakshmi Pat Singhania-IIM Lucknow National Leadership Awards 2011 (Young Leader)
6. Under Eureka programme, [Interview was telecast at Rajya Sabha TV Channel \(RTV\)](#), in 2015
7. Felicitated by Chief Minister of Uttar Pradesh (UP) at occasion of UP Diwas (26th Jan 2018) for significant contribution in the field of Bioinformatics.
8. Sun Pharma Research Award 2018 by Sun Pharma Science Foundation
9. Scientist Award 2019 by Organization of Pharmaceutical Producers of India
10. Distinguished Alumni Award for the year 2025 by IIT Delhi

➤ **Major citation-based international recognitions**

1. Highly Cited Researcher in the field of Computer Science – 2014 by Thompson Reuters. Listed in "[The World's Most Influential Scientific Minds](#)" that contains highly cited 3200 individuals whose papers rank in the top 1% by citations in their field and year of publication. Seven Indian scientists have been listed in above list.
2. [Thomson Reuters Research Excellence](#) - India Research Front Awards 2009 as two of his papers ranked in the category of highly cited papers in the world.
3. Ranked #4 globally in Bioinformatics as per ScholarGPS and is consistently listed among the Top 0.05% of Scientists worldwide across all disciplines.
4. One paper listed in top 70 highly cited papers (ranked 18) published by CSIR scientists in last 70 years
5. In the list of [top 2% highly cited researchers](#) in the world, in the field of Bioinformatics, This list is based on study [PLoS Biol 18\(10\): e3000918](#).
6. Ranked 5<sup>th</sup> in the list of [highly cited Indian researchers](#) in the field of Biology and Biochemistry.
7. Ranked 3<sup>rd</sup> in India and 456<sup>th</sup> in world as per AD Scientific index in the field of computer science see [https://www.adscientificindex.com/scientist\\_print.php?id=394479](https://www.adscientificindex.com/scientist_print.php?id=394479)

➤ **Other awards and recognitions**

1. Teach Excellence awards by IIT Delhi
2. Outstanding educator award by IIT Delhi
3. Institute Chair Professor by IIT Delhi
4. Lifetime Achievement Award 2024 by Bioclues
5. Outstanding Contribution to National Development (OCND) Award for year 2025 by IIT Delhi Alumni Association
6. Lifetime achievement award 2025 by Bioinformatics and Drug Discovery Society.

## SCIENTIFIC JOURNEY

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Prof. Gajendra Pal Singh Raghava, a pioneer in Indian bioinformatics, has devoted over three decades to advancing computational biology, with a mission to create accessible, open-source resources for the global scientific community. His career is marked by a rare blend of innovation, service, and leadership that has significantly shaped bioinformatics and translational medicine in India and beyond.

**Early Education and Transition to Bioinformatics:** Born in 1963 in Bulandshahr, Uttar Pradesh, Prof. Raghava pursued an M.Sc. in Physics from Meerut University (1984) and an M.Tech. in Energy Studies from the Indian Institute of Technology, Delhi (1986). At IIT Delhi, his passion for computing took shape, leading him to design microprocessor-based real-time applications for process control.

In 1986, he joined the Council of Scientific and Industrial Research's Institute of Microbial Technology (CSIR-IMTECH), Chandigarh, as a Computer Scientist. Initially focused on software for scientific management, he soon turned his attention to solving pressing biomedical challenges. In 1990, he developed a novel program for quantifying antibodies and antigens from ELISA data, which proved more accurate than existing software and was validated experimentally. A resulting publication in the Journal of Immunological Methods marked his entry into bioinformatics and set the tone for a career devoted to providing computational solutions to the life sciences community.

**Growth of Bioinformatics Research:** Recognizing the importance of open science, Prof. Raghava freely shared his software tools, establishing himself as a researcher committed to community-driven science rather than individual recognition. To broaden India's visibility in global bioinformatics, he actively participated in international challenges such as CASP (Critical Assessment of Protein Structure Prediction), DREAM Challenges, and Kaggle competitions. His international engagements included a postdoctoral fellowship at Oxford University, UK (1996–1998), establishing bioinformatics centers at the University of Arkansas for Medical Sciences, USA (2002 and 2006), and a visiting professorship at POSTECH, South Korea (2014). Despite multiple offers abroad, he chose to dedicate his career to building bioinformatics capacity in India.

**Building a Research Legacy at IMTECH:** In 2000, Prof. Raghava formally established his research group at IMTECH, focusing on the annotation of genomes and proteomes. His team pioneered computational methods for predicting protein structure and function, particularly in the area of subcellular localization. His outstanding contributions earned him the DBT National Bioscience Award in 2006. As a leader in the CSIR "In Silico Drug Targets" project, he advanced methods to identify novel drug and vaccine candidates, work that was recognized with the prestigious Shanti Swarup Bhatnagar Prize in Biological Sciences (2008). In 2007, he played a pivotal role in CSIR's ambitious "Open Source Drug Discovery (OSDD)" initiative, aimed at reducing drug development costs for diseases such as tuberculosis. His group developed and maintained the in silico module, "Computational Resources for Drug Discovery (CRDD)," and created OSDDLlinux, a specialized Linux-based platform integrating bioinformatics software. These open-source resources had significant economic impact, particularly for researchers in developing nations. In recognition, he was awarded the J. C. Bose National Fellowship by DST in 2010.

**Bridging In Silico and Experimental Research:** In 2012, Prof. Raghava established an experimental laboratory to complement computational work with experimental validation. His group discovered novel cell-penetrating peptides (CPPs) and drug delivery vehicles, demonstrating their ability to transport therapeutic molecules into cells and across the skin barrier. Importantly, these vehicles were shown to overcome drug resistance by enabling drugs to cross bacterial membranes. This translational success was recognized with the Sun Pharma Research Award in 2018.

**Leadership at IIIT Delhi:** In 2017, Prof. Raghava joined the Department of Computational Biology at Indraprastha Institute of Information Technology (IIIT), Delhi, as Professor (HAG). His research has since focused on genomics-driven approaches to understand and manage complex diseases, particularly cancer. His group developed innovative tools to predict biomarkers for cancer diagnostics, prognosis, and therapy selection. This work earned him the Scientist of the Year award from the Organisation of Pharmaceutical Producers of India in 2019. Today, Prof. Raghava leads one of the most widely used bioinformatics groups worldwide. His team has developed over 300 databases and web servers, freely available for academic use, serving more than 200,000 users daily and saving the research community an estimated ₹200 crore annually in software costs.

**Philosophy and Impact:** Throughout his career, Prof. Raghava has remained guided by a philosophy of inclusivity and service. His approach—engaging directly with experimental biologists, understanding their challenges, and translating them into computational solutions—has made his work deeply relevant and impactful. By consistently choosing open access over commercialization, he has ensured that researchers, particularly in resource-limited settings, can benefit from cutting-edge bioinformatics tools. His scientific journey reflects not only academic excellence but also a commitment to national development, global collaboration, and societal benefit. Prof. Raghava continues to inspire a new generation of computational biologists, demonstrating how science, when pursued with vision and service, can transform both knowledge and society.

## RESEARCH PUBLICATIONS

**Major Publications:** 227 (Publications in reputed journals as a corresponding author, see **Annexure I**), Following is list of few journals where papers have been published

Name of Journal	Impact Factor*	No. of Papers	Total Impact	Comment
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Nucleic acids research	19.2	16	307	*Impact factor is either latest if paper published long time back or maximum impact factor if multiple papers published in different years.  *Total Impact Factor of all papers (corresponding author) is <b>1382</b>
Briefings in Bioinformatics	14.0	11	154	
Genome Research	14	1	14	
Bioinformatics	6.9	11	76	
Computers in Biology and Medicine	7.0	11	77	
Database (Oxford)	4.5	10	45	
Journal Biol. Chemistry	6.4	3	19	
Drug Discovery Today	7.8	4	31	
BMC Bioinformatics	5.4	20	108	
Proteomics	5.4	7	38	
Scientific Reports	5.6	23	123	
Other Papers	~3.2 (Avg)	125	384	
<b>Total</b>		<b>236</b>	<b>1382</b>	

**Other peer reviewed publications:** 84 papers (collaborative papers, papers in low impact factor journals, consortium paper, non-corresponding author papers). Total impact factor is around 400, See **Annexure II**

**Chapters in reputed books/protocols:** 18 (See **Annexure III**)

## CITATION INFORMATION

**Citation Information (Google Scholar):** As per google scholar, total citation is around 31760 with h-index 92. Corresponding author in 90 out of 100 highly cited papers; corresponding author of top 15 highly cited papers. Following is citation information as per google scholar

Citation Summary	
Total citations on all papers	34000
Total citations in last five years	19000
Maximum citation of a single paper	1900
Papers with more than 300 citations	37
Papers with more than 200 citations	46
Papers with more than 100 citations	89
Papers with more than 10 citations (g-index)	287
Average Citation per paper	~90
h-index	94

## PATENTS AND COPYRIGHTS

**Patents:** 3 (List is given below)

1. Raghava GPS, Gautam A, Nandanwar HS (2015): Cell Penetrating Peptide for Biomolecule Delivery. Patent WO/2015/075747-A1 .

2. Raghava GPS, Gautam A (2018): Chemically Modified Cell-penetrating peptide for Intracellular Delivery of Nucleic Acids. WO/2018/173077.
3. Sharma DK, Gupa A, Raghava GPS, Gautam A, Kumari M (2019) Potent Peptide Inhibitors of Protein Aggregation. WO/2019/058389
4. Sharma DK, Gupta A, Raghava GPS, Gautam A, Kumari M (2023) Potent Peptide Inhibitors of Protein Aggregation. US: 16647149.

**Copyrights:** 70 (Copyrights have been taken on standalone software packages and websevers.) See Annexure IV

## MAJOR PROJECTS/FUNDINGS

### (Major grants/projects as project leader/coordinator)

**1) Bioinformatics Centre on Protein Modelling/Engineering (Coordinator: G. P. S. Raghava):** A continuous project of Department of Biotechnology, Govt. of India, to provide bioinformatics services at national level. The Bioinformatics Center at Institute of Microbial Technology, Chandigarh was established in 1987 with specialization in the area of Protein Modeling and Protein Engineering. This is one of the core facilities in the field of biotechnology providing access to the latest information of the worlds databases in the fields of Protein Modeling and Protein Engineering. Dr. Raghava headed this project from 1994 to 2017, securing funding of approximately Rs 5 crores from the Department of Biotechnology.

**2) Genomics and Informatics Solutions for integrating Biology (GENESIS):** This was a mega network project of CSIR under 12th five-year plan (2012-2017) where Raghava is nodal officer. In this project 15 CSIR labs and nearly 55 scientists are participated in this project. GENESIS is an interdisciplinary project which aims to integrate computational scientists and biologists across CSIR to understand complex biological problems, mathematically model biological systems, compile and mine experimental data, discover drug/vaccine candidates and finally support translation of leads to medicine. This project total budget was around Rs 50 crores.

**3) Advanced Centre for Protein Informatics, Science, Engineering & Technology (2007-2011):** This is a facility creation project of CSIR, coordinated by CSIR-IMTECH (Nodal Officer: G P S Raghava) under 11th five-year plan. Aim of this project was to set up a one-stop Centre for expertise, consultancy, and facilities, in the area of protein science and engineering, and protein biotechnology. This project has been completed successfully with world class infrastructure for Protein Informatics, Science, Engineering & Technology. Raghava got total fund of around 40 crores under this project.

**4) J. C. Bose national fellowship:** Raghava got this prestigious fellowship for 2010-2015 and 2015-2020 from department of science and technology (DST). Aim of this fellowship/project is to understand biological interactions particularly interaction network of proteins. Total for two tenure of this fellowship is more than 1.5 cores.

**5) Establishment of Bioinformatics and Computational Biology Centre (2021-2026):** Department of biotechnology, Govt. of India is establishing bioinformatics centres in India to promote. Under this programme, department of computational biology (IIITD) applied for a project under leadership of Dr Raghava to establish bioinformatics centre at IIIT Delhi. Department of biotechnology sanction a project of worth Rs 1.56 crore to IIIT Delhi for five years to establish bioinformatics centre.

**6) Development of Multi-domain reliable reproducible and robust platform for Research in Bioinformatics (2022-2027):** This is a multi-institute project where six national institutes (IIIT Delhi, IGIB, JNU, ICGEB, NIPGR, DU South Campus) are collaborating to develop protocol for unified web-based platform. This project is funded by Department of Biotechnology, Govt. of India (project approved). This project is lead by IIIT Delhi under leadership of Dr Raghava. This is a five-year project with budget around 2.5 Lakhs.

## RESEARCH CONTRIBUTION

### Significant contributions to science and/or technology

Raghava is a highly original and dedicated bioinformatician, who has developed numerous algorithms to provide computer-based solutions in the field of life/health sciences. In contrast to traditional researchers where a scientist contributes to a particular problem or field; He contributed to multiple problems/fields important for translational

medicine. His group mainly focuses on data intensive research for mining important information and rule from wide range of biological data. Following are highlight of his scientific contributions.

**Database Development:** To establish a solid foundation for data-intensive research, our group has developed over fifty exceptional primary databases in the healthcare field. These databases house meticulously curated, experimentally validated data extracted from literature and other sources. Both experimentalists and informatics specialists heavily rely on these databases for their work. It is worth noting that all of these databases have been published in renowned journals and are extensively utilized by the scientific community to advance knowledge-based methodologies. According to the "[Database Commons](#)" India holds an impressive third position in terms of the number of developed databases, most of the databases developed by our group.

**Computer-Aided Vaccine Design:** Raghava's group is working in the field of vaccine informatics from last 20 years in order to understand the immune system to design effective vaccines. More than 50 web-servers have been developed for predicting peptides that induce both arm of immune system; adaptive and innate immune system. Group is actively working to design computer-aided vaccine candidates to fight against wide range of infectious. Six primary/reference immunological databases (MHCBN, BCipep, PRRDB, AntigenDB, HaptenDB, PolysacDB) have been developed by his group. In order to provide comprehensive solutions for vaccine development, group developed methods for predicting vaccine targets that includes B-cell, T-cell and A-cell (vaccine adjuvants) epitopes. In order to compute ADMET properties of peptides, methods have been developed for predicting toxicity, half-life, hemotoxicity and cell-penetrating peptides.

**Potential Drug Targets:** His group developed software for annotating genomes at nucleotide as well as at protein level, in order to identify potential drug targets. Number of novel methods have been developed for identifying potential drug targets that includes receptors, toxins and virulent proteins. In order to develop drugs against these targets, algorithms have been developed for predicting secondary, super secondary structure (e.g. beta-hairpins, beta-barrels) and tertiary structure of these targets proteins. The performance of their best secondary structure prediction method was ranked within the top methods in the world.

**Need-based Solutions:** One of the unique feature of his group is that group provides solutions for complicated and emerging problems face by society. Recently, group developed number in silico platforms for providing bioinformatics based solutions for managing different diseases. CancerDP is a web-based service developed for selecting right drug for right person based on their genome sequence. MtbVeb is a web-based platform developed for designing vaccines and immunotherapy against existing, emerging and drug-resistant strains of mycobacterium tuberculosis. This includes drug resistant and extreme drug resistant M. Tb strains. Ebola Virus Computational Resources (EbolaVCR) is the in silico resources developed to facilitate scientific community fighting against deadly virus Ebola. CoronaVIR developed for compiling computational resources on coronavirus to facilitate the scientific community to fight against severe pandemic disease COVID-19 caused by SARS-CoV-2.

**Personalized/Strain specific Medicines:** In the era of next generation sequencing where sequencing of whole genome of pathogens (bacteria/fungus/virus) and human is affordable; it is important to develop person or strain-specific medicine. His group have already sequenced, assembled and annotated whole genome of more than 15 bacterial and fungal organisms. Raghava group is in the process of developing *in silico* tools for personalized medicine; following are major resources developed in last few years; a) [HIVcoPred](#): Prediction HIV-1 coreceptor from its V3-loop sequence; b) [DipCells](#): Promiscuous inhibitors against pancreatic cancer cell-lines; c) [HerceptinR](#): Herceptin resistance database against various cancer cell-lines with genomic information and d) [PCMDB](#): methylation information about important genes across various pancreatic cell lines and tissues.

**Computational Resources for Drug Discovery:** Despite the tremendous progress in the field of drug designing, discovering a new drug molecule is still a challenging task. Drug discovery and development is a costly, time consuming and complex process that requires millions of dollar and 10-15 years to bring new drug molecules in the market. In addition proprietary nature of processes involved in drug discovery further increase the cost of drugs. In 2008, CSIR has taken an initiative called 'Open Source Drug Discovery (OSDD)' in order to provide affordable healthcare. Its major aims to synergize the power of genomics, computational technologies and facilitate the

participation of young and brilliant talent from Universities and industry. Under OSDD, Raghava's group developed and maintain Insilco module of OSDD called "Computational Resources for Drug Discovery (CRDD)". Under CRDD all the resources related to computer-aided drug design(CADD) have been collected and compiled at a single platform Major initiatives have been taken to bring down the cost of CAAD software by developing open source in the field of drug discovery.

**Experimental Validation of Predictions:** In addition to software/webserver/database development, his group also established experimental lab to validated in silico predictions in wet-lab. Aim was to discover novel drug delivery vehicles using combination of in silico and experimental techniques. In 2012, his group developed a database CPPsite to maintain cell penetrating peptides (CPPs) that can be used to deliver drug inside a cell. These CPPs were mined using machine learning techniques to develop computational method CellPPD for predicting cell penetrating peptides. In order to discover highly effective CPPs, all proteins in Swissport database were scanned using CellPPD and identified ten peptides having highest CPP potential. These predicted experimental peptides were experimentally tested on different cell lines. This leads to discovery of experimentally validated novel drug delivery vehicles. These vehicles not only deliver drugs inside cell even they can be used to deliver drug via skin (topical drug delivery). His lab also demonstrate that drug delivery vehicles can be used to handle drug resistant bacteria as it facilitates drugs to cross membrane of bacteria.

## TEACHING AND HUMAN RESOURCE DEVELOPMENT (HRD)

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Raghava works at two organization (CSIR-IMTECH and IIIT Delhi), following is brief description of contribution at two organizations.

- **Long term training:** More than 500 students have been trained (PA, RA, Summer trainees) that includes 55 Ph.D students (41 completed).
- **Short Training:** More than 800 students got short term training as workshop/conference participants. Two international & more than 10 national workshop/training/conference were organized.
- **Bioinformatics Course:** Taught around 200 pre-phd students over the years; full one session. In addition, we are organizing small training programs for faculty and student of IMTECH from last 20 years.
- **Virtual skill development:** In addition to direct training, we are providing training to users via our online computational resources. All tutorials/ documents/presentations related to bioinformatics are available from our sites. Under GPSR package we provide PERL code required to write core script in the field of computational biology. All over the world students and young faculties are using theses source codes for learning as well as for developing their own software packages.
- **Specialized Trainings:** A customized training was organized for employees of a private company from South Korea in the year of 2002, for which we received Rs 4.55 lakhs. We also organized training for Department of Electronics (DOE) in year 2003, on PERL in Bioinformatics for which we received Rs 2.80 lakhs.
- **Courses Taught:** Since 2017, Raghava is working at IIIT Delhi, he taught two courses ("Machine Learning for Biomedical Applications" and "Big Data Mining in Healthcare"), both courses are popular among students ( more than 150 students per batch).

## SERVICE CONTRIBUTIONS

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### Institute service

- Number of workshop/conferences organized at department of computational biology at IIIT Delhi.
- Serving as Head of Department and contributing to all department activities
- Member/chairman of number of committees at IIIT Delhi including chairman of space committee.
- Contributed towards for initiating B. Tech in Computer Science and Bioscience program at IIIT Delhi in year 2018.

### Service outside the institute / Professional Service

- Role as Editor: Serving editor in reputed journals like Section Editor of Translational Medicine, Academic Editor of Plos One, Associate Editor of BMC Bioinformatics.
- Role as Reviewer: Reviewed number of manuscript for reputed journals.
- Number of Ph.D. thesis has been evaluated for reputed universities.
- Number of invited lectures have been delivered in workshops/conferences.
- Serving as a member of Task Force on “Theoretical and computational Biology” of DBT.

### Service for Society

- **Portal for Health Informatics (PHI):** A web portal “Portal for Health Informatics (PHI)” has been developed to compile contribution of Indian Researchers/Academicians in the field of health informatics (See <http://webs.iiitd.edu.in/> ). This web portal maintained wide range of servers, databases and software developed in the field of bioinformatics, chemoinformatics, immunoinformatics, clinical bioinformatics, health informatics, genomics, etc.
- **Group Web Server at IIITD:** This was the first major project for group to install/launch web servers developed by group in the last two decades. We successfully install and set more than 300 web servers at IIIT at Delhi. All web servers including new web servers developed at IIIT Delhi are working fine and heavily used by the scientific community. Scientific community especially experimental researcher are using our web server for predicting and validating vaccine and drug targets ( <http://webs.iiitd.edu.in/raghava/> ).

## TECHNOLOGY DEVELOPMENT

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### Social Impact of Technologies

Raghava group has developed number of web services (servers and databases), each service is based on novel algorithm or data and has been published in reputed journals. Most of publications based on these services are highly cited. His group developed more than 300 insilico products (web servers, databases and software packages) which is highest contribution by a single group in the world. Raghava is strong supporter of open source software/web-servers; all service developed at his group are free for academic use. These web-based services are heavily used worldwide, more than 200,000 hits per day. In 2015, impact of his services was computed based on cost of equivalent commercial software packages in market, it was found that group is providing service of worth Rs 200 crore per year (See Annexure V for detail). In last eight years number of services increased from 200 to 300. Raghava got following major awards and recognitions based on technologies developed in his group

- **Delivery of Drugs via Skin:** One of the major challenge in drug discovery is to deliver a drug molecule at right target (inside a cell) particularly through topical route (skin). Raghava's group compile all peptides from literature whose potential to penetrate cell/skin have been validated experimentally. This knowledge-base has been used to develop AI based models for predicting cell penetrating peptides. These AI models were used to discover novel cell/skin penetrating peptide, which were validated experimentally (in vitro and animal models). It was demonstrated that these peptides are better than any existing cell penetrating peptide, can deliver drug inside cell, can deliver drug via skin.

**Outcome:** 3 patents, AI based prediction servers, 10 research papers

**Recognition of work:** Sun Pharma Research Award 2018 (2.5 lakhs); OPPI Scientist Award 2019 (Rs 1 lakh)

- **AI based models for designing vaccines:** Scientific community fails to design vaccine against number of dread viruses and bacteria due to the limitation of traditional vaccine candidates. Due to advancement of technology, there is an exponential growth of data in the field of vaccine biology. Raghava's group fully utilize this data to develop AI based models for predicting wide range of functions of immune system for designing effective vaccines. In order to facilitate community, he integrate these models in web based products.



**Outcome:** 30 Copyrights; ~50 Web servers; ~70 research papers

**Recognition:** Shanti Swarup Bhatnagar Award, NASI-Reliance Industries Platinum Jubilee Award (3 lakhs), JC Bose National Fellowship.

- **In silico tools for cancer biomarkers:** There are number of challenges in managing cancer treatment that includes identification of cancer in early stage, stage of cancer, risk of cancer. Raghava's group have developed number of AI based prediction models using genomic features of cancer patients and health individuals. These models are available to public in form on web based products, it includes prediction of early stage cancer patients, high risk patients, stage of cancer, progression of cancer in tissue.

**Outcome:** 25 research papers, 20 web-based services

### **Commercialized products**

- Contributed in the development of BioSuite which is a bioinformatics software developed by Tata Consultancy Services (TCS) with experts in bioinformatics under the NMITLI programme. Hon'ble President of India Dr APJ Abdul Kalam launched this package on 14<sup>th</sup> July 2004.
- In collaboration with a private company, Biomantra, our group developed a software package. This software, "VaxiPred: Computer aided vaccine design", was based on research carried out at my group. CSIR Director General, Dr R A Mashlekar has launched this package on 15<sup>th</sup> December 2004.

## Major Publications

(Papers in Reputed Journals; Corresponding Author in all papers)

1. Gahlot P, Choudhury S, Bajiya N, Kumar N, Raghava GP (2024) Prediction of plant resistance proteins using alignment-based and alignment-free approaches. **Proteomics** (In Press)
2. Dhall A, Patiyal S, Raghava GP (2024) A hybrid method for discovering interferon-gamma inducing peptides in human and mouse. **Sci Rep.** 14(1):26859.
3. Patiyal S, Dhall A, Kumar N, Raghava GP (2024) HLA-DR4Pred2: An improved method for predicting HLA-DRB1\*04:01 binders. **Methods.** 232:18-28.
4. Kumar N, Choudhury S, Bajiya N, Patiyal S, Raghava GP (2024) Prediction of Anti-Freezing Proteins From Their Evolutionary Profile. **Proteomics.** e202400157.
5. Patiyal S, Tiwari P, Ghai M, Dhapola A, Dhall A, Raghava GP (2024) A hybrid approach for predicting transcription factors. **Front Bioinform.** 4:1425419.
6. Rathore AS, Choudhury S, Arora A, Tijare P, Raghava GP (2024) ToxinPred 3.0: An improved method for predicting the toxicity of peptides. **Comput Biol Med.** 179:108926
7. Jarwal A, Dhall A, Arora A, Patiyal S, Srivastava A, Raghava GP (2024) A deep learning method for classification of HNSCC and HPV patients using single-cell transcriptomics. **Front Mol Biosci.** 11:1395721.
8. Jain S, Gupta S, Patiyal S, Raghava GP (2024) THPdb2: compilation of FDA approved therapeutic peptides and proteins. **Drug Discov Today.** 29(7):104047.
9. Kaur D, Arora A, Vigneshwar P, Raghava GP (2024) Prediction of peptide hormones using an ensemble of machine learning and similarity-based methods. **Proteomics.** 24(20):e2400004.
10. Bajiya N, Choudhury S, Dhall A, Raghava GP. (2024) AntiBP3: A Method for Predicting Antibacterial Peptides against Gram-Positive/Negative/Variable Bacteria. **Antibiotics** 13, 168.
11. Choudhury S., Bajiya N., Patiyal S. and Raghava GP. (2024) MRSLpred -A hybrid approach for predicting multi-label subcellular localization of mRNA at genome scale. *Front. Bioinform.* doi: 10.3389/fbinf.2024.1341479.
12. Kumar N, Tripathi S, Sharma N, Patiyal S, Devi NL, Raghava GP. (2024) A method for predicting linear and conformational B-cell epitopes in an antigen from its primary sequence. *Comput Biol Med.* 170:108083.
13. Dhall A, Patiyal S, Kaur H, Raghava GP. (2023) Risk assessment of cancer patients based on HLA-I alleles, neobinders and expression of cytokines. *Comput Biol Med.* 167:107594.
14. Kumar N, Bajiya N, Patiyal S, Raghava GP. (2023) Multi-perspectives and challenges in identifying B-cell epitopes. *Protein Sci.* 32(11):e4785.
15. Arora A, Patiyal S, Sharma N, Devi NL, Kaur D, Raghava GP. (2023) A random forest model for predicting exosomal proteins using evolutionary information and motifs. *Proteomics.* e2300231.
16. Tripathi, S., Sharma, N., Devi, N.L., and Raghava, G.P. (2023). ViralVacDB: a manually curated repository of viral vaccines. **Drug Discovery Today**, 103523.
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## Other Peer Review Publications

(Consortium/collaborative/non-corresponding author papers and publications in low impact factor journals)

1. Priyadarsinee et al. (2024) Molecular Property Diagnostic Suite for COVID-19 (MPDS<sup>COVID-19</sup>): an open-source disease-specific drug discovery portal. *GigaByte*. 2024 Mar 14;2024:gigabyte114.
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## Social Impact of Web Services Developed by Raghava's Group

Group have developed number of web services (servers and databases), each service is based on novel algorithm or data, published in reputed journals. Most of publications based on these services are highly cited. Scientific community in the field of education, vaccine and drug discovery heavily uses these services. Following is procedure used to calculate social impact on society.

1. Hits per year for 125 services is computed from Apache log of six months
2. Total hits per server are computed by multiplying per year hits with time (years) service is online.
3. Number of scientific pages visited and job submitted were computed by dividing hits by factor of three and six respectively.
4. Social impact is computed by charging Rs 5 for visiting a scientific page and Rs 500 for executing/submitted a job.

**Total social impact in term money is around Rs. 792 crore in year 2015**

(Detail is given in table below)

Web-Servers	Online (Years)	Hits/year	Total hits	Pages/visited	Jobs executed	Social Impact (Rs in lakhs)
dnabinder	9	1218502	10966518	3655506	1827753	9321
pcmdb	3	2387778	7163334	2387778	1193889	6088
metapred	6	929140	5574840	1858280	929140	4738
mhcbn	13	366192	4760496	1586832	793416	4046
rnapred	7	633188	4432316	1477438	738719	3767
cancerdr	4	916792	3667168	1222389	611194	3117
cppsite	4	762016	3048064	1016021	508010	2590
bcepred	13	214590	2789670	929890	464945	2371
sarpred	11	232384	2556224	852074	426037	2172
proprint	8	292022	2336176	778725	389362	1985
lbtope	3	774590	2323770	774590	387295	1975
propred	14	155590	2178440	726146	363073	1851
pepstr	9	229592	2066328	688776	344388	1756
hmrbase	8	247044	1976352	658784	329392	1679
npact	3	499456	1498368	499456	249728	1273
glycoep	3	484306	1452918	484306	242153	1234
abcpred	10	139888	1398880	466293	233146	1189
ccpdb	4	332040	1328160	442720	221360	1128
npred	7	189214	1324498	441499	220749	1125
hslpred	12	107388	1288656	429552	214776	1095
apssp	15	77752	1166280	388760	194380	991
cancerppd	2	562058	1124116	374705	187352	955
eslpred	12	93444	1121328	373776	186888	953
antigendb	6	172270	1033620	344540	172270	878
rnacon	4	257562	1030248	343416	171708	875
bcipep	12	83396	1000752	333584	166792	850
btcpred	10	99834	998340	332780	166390	848

dipcell	2	459386	918772	306257	153128	780
hemolytik	3	275756	827268	275756	137878	703
propred1	13	62924	818012	272670	136335	695
haptendb	12	62870	754440	251480	125740	641
algpred	9	72116	649044	216348	108174	551
polyapred	7	92420	646940	215646	107823	549
ctlpred	11	58078	638858	212952	106476	543
Ccdb	5	124528	622640	207546	103773	529
biadb	6	102020	612120	204040	102020	520
betatpred	13	43472	565126	188375	94187	480
tumorhope	4	138970	555880	185293	92646	472
Ftg	14	36358	509012	169670	84835	432
herceptinr	3	169462	508386	169462	84731	432
antibp	9	53776	483984	161328	80664	411
alphapred	12	36738	440856	146952	73476	374
ahtpdb	1	426226	426226	142075	71037	362
betaturns	12	35518	426216	142072	71036	362
nhlapred	11	37572	413292	137764	68882	351
toxipred	5	76006	380030	126676	63338	323
mitpred	8	46524	372192	124064	62032	316
betatpred3	1	366568	366568	122189	61094	311
betatpred2	12	30144	361728	120576	60288	307
tappred	12	30142	361704	120568	60284	307
rslpred	8	44148	353184	117728	58864	300
pslpred	11	31550	347050	115683	57841	294
polysacdb	6	55904	335424	111808	55904	285
pprint	8	41228	329824	109941	54970	280
eslpred2	8	39568	316544	105514	52757	269
rbpred	9	30562	275058	91686	45843	233
parapep	3	89468	268404	89468	44734	228
anticp	3	87962	263886	87962	43981	224
tbbpred	12	21154	253848	84616	42308	215
cellppd	3	82646	247938	82646	41323	210
mmbpred	13	17678	229814	76604	38302	195
ntegfr	2	109954	219908	73302	36651	186
egpred	12	18014	216168	72056	36028	183
antibp2	7	30174	211218	70406	35203	179
gpcrpred	12	17118	205416	68472	34236	174
gammapred	12	15542	186504	62168	31084	158
bteval	12	14552	174624	58208	29104	148
srtpred	8	21758	174064	58021	29010	147
chpredict	14	12348	172872	57624	28812	146
igpred	4	43030	172120	57373	28686	146
vicmpred	7	24384	170688	56896	28448	145
gwbblast	11	15240	167640	55880	27940	142
cbtope	6	27918	167508	55836	27918	142

glycopp	4	41256	165024	55008	27504	140
gwfasta	12	13514	162168	54056	27028	137
toxinpred	4	39726	158904	52968	26484	135
hivsir	5	30070	150350	50116	25058	127
Gdoq	8	17854	142832	47610	23805	121
rnapin	3	46612	139836	46612	23306	118
kidoq	7	18914	132398	44132	22066	112
egfrindb	2	65730	131460	43820	21910	111
ifnepitope	3	40010	120030	40010	20005	102
proglycprot	5	23866	119330	39776	19888	101
drugmint	3	36518	109554	36518	18259	93
trnamod	2	52068	104136	34712	17356	88
pcleavage	10	9950	99500	33166	16583	84
ntxpred	9	10900	98100	32700	16350	83
phdcleav	6	15324	91944	30648	15324	78
prbdb	9	10216	91944	30648	15324	78
desirm	5	17962	89810	29936	14968	76
ar_nhpred	12	7452	89424	29808	14904	76
nrpred	13	6368	82784	27594	13797	70
bhairpred	11	7504	82544	27514	13757	70
atpint	7	10556	73892	24630	12315	62
vgichan	9	7076	63684	21228	10614	54
tumorhpd	4	15684	62736	20912	10456	53
egfrpred	2	29308	58616	19538	9769	49
pseapred	8	6662	53296	17765	8882	45
icaars	5	10362	51810	17270	8635	44
dmkpred	5	9452	47260	15753	7876	40
gpcrsclass	10	4618	46180	15393	7696	39
Hlp	2	22370	44740	14913	7456	38
nadbinder	6	7350	44100	14700	7350	37
gstpred	8	5444	43552	14517	7258	37
pfmpred	7	5882	41174	13724	6862	34
premier	6	6628	39768	13256	6628	33
cancer_pred	5	7558	37790	12596	6298	32
gtpbinder	7	5040	35280	11760	5880	29
oxypred	9	3868	34812	11604	5802	29
vitapred	3	11376	34128	11376	5688	29
Mdri	4	8440	33760	11253	5626	28
ahtpin	1	32314	32314	10771	5385	27
oxdbase	7	4538	31766	10588	5294	26
cytopred	8	3810	30480	10160	5080	25
il4pred	3	8942	26826	8942	4471	22
marspred	4	6682	26728	8909	4454	22
dprot	8	3286	26288	8762	4381	22
hivcopred	3	7694	23082	7694	3847	19
chemopred	7	2888	20216	6738	3369	17

vaccineda	1	17388	17388	5796	2898	14
fadpred	6	2682	16092	5364	2682	13
xiapin	1	13030	13030	4343	2171	11
paaaint	2	4988	9976	3325	1662	8
antiangiopred	1	8356	8356	2785	1392	7
<b>Total</b>	<b>880</b>	<b>16993588</b>	<b>93216050</b>	<b>31071990</b>	<b>15535982</b>	<b>79233</b>