

# Curriculum Vitae

Gajendra P. S. Raghava

## PERSONAL DETAILS

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

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

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

Email: [ragahva@iiitd.ac.in](mailto:ragahva@iiitd.ac.in)

Current Position: **Professor**

Organization/Institute: **IIIT, Delhi**

Google Scholar: [XK5GUiYAAAAJ](https://scholar.google.com/citations?user=XK5GUiYAAAAJ)

## 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

From	To	Place of Employment	Designation	Scale of Pay
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	PB IV 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

From	To	Institute/ country visited	Purpose of visit
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 Carrier 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 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 who's papers rank in the top 1% by citations in their field and year of publication. Seven Indian scientist 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 IIIT Delhi
2. Outstanding educator award by IIIT Delhi
3. Institute Chair Professor by IIIT 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**

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 OSDDlinux, 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
-----------------	----------------	---------------	--------------	---------

Nucleic acids research	19.2	16	307	<p>*Impact factor is either latest if paper published long time back or maximum impact factor if multiple papers published in different years.</p> <p>*Total Impact Factor of all papers (corresponding author) is <b>1382</b></p>
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, IIGB, 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 (MHCDB, BCIpep, PRRDB, AntigenDB, HapteneDB, 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 validate 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)

---

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 these 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

---

### 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**

---

### **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 woth Rs 200 crore per year (See Annexure V for detail). In last eight years number of sevices 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, Bajiy 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, Bajiy 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. Bajiy 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., Bajiy N., Patiyal S. and Raghava GP. (2024) MRSpred -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, Bajiy 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.
17. Patiyal, S., Dhall, A., Bajaj, K., Sahu, H., and Raghava, G.P. (2023). Prediction of RNA-interacting residues in a protein using CNN and evolutionary profile. **Briefings in Bioinformatics** 24, bbac538.
18. Naorem, L.D., Sharma, N., and Raghava, G.P. (2023). A web server for predicting and scanning of IL-5 inducing peptides using alignment-free and alignment-based method. **Computers in Biology and Medicine** 158, 106864.
19. Kaur, D., Arora, A., Patiyal, S., and Raghava, G.P.S. (2023). Hmrbase2: A comprehensive database of hormones and their receptors. **Hormones**, 22(3):359-366.
20. Dhall, A., Patiyal, S., Choudhury, S., Jain, S., Narang, K., and Raghava, G.P. (2023). TNFepitope: A webserver for the prediction of TNF- $\alpha$  inducing epitopes. **Computers in Biology and Medicine** 160, 106929.
21. Arora, A., Kaur, D., Patiyal, S., Kaur, D., Tomer, R., and Raghava, G.P. (2023). SalivaDB—a comprehensive database for salivary biomarkers in humans. **Database** 2023, baad002.
22. Tomer, R., Patiyal, S., Dhall, A., and Raghava, G.P. (2023). Prediction of celiac disease associated epitopes and motifs in a protein. **Frontiers in Immunology** 14.
23. Aggarwal, S., Dhall, A., Patiyal, S., Choudhury, S., Arora, A., and Raghava, G.P. (2023). An ensemble method for prediction of phage-based therapy against bacterial infections. **Frontiers in Microbiology** 14, 1148579.
24. Sharma, N., Naorem, L.D., Jain, S., and Raghava, G.P. (2022). ToxinPred2: an improved method for predicting toxicity of proteins. **Briefings in Bioinformatics** 23, bbac174.
25. Roy, T., Sharma, K., Dhall, A., Patiyal, S., and Raghava, G. (2022). In silico method for predicting infectious strains of influenza A virus from its genome and protein sequences. **J Gen Virol.** 103, 11.

26. Sharma, N., Naorem, L.D., Gupta, S., and Raghava, G.P. (2022). Computational resources in healthcare. *Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery* 12, e1437.
27. Patiyal, S., Singh, N., Ali, M., Pundir, D., and Raghava, G. (2022). Sigma70Pred: A highly accurate method for predicting sigma70 promoter in *Escherichia coli* K-12 strains. *Frontiers in Microbiology* 13 doi.org/10.3389/fmcb.2022.1042127.
28. Patiyal, S., Dhall, A., and Raghava, G.P. (2022). A deep learning-based method for the prediction of DNA interacting residues in a protein. *Briefings in Bioinformatics* 23, bbac322.
29. Kumar, N., Patiyal, S., Choudhury, S., Tomer, R., Dhall, A., and Raghava, G.P. (2022). DMPPred: a tool for identification of antigenic regions responsible for inducing type 1 diabetes mellitus. *Briefings in Bioinformatics* 23, bbac525.
30. Jain, S., Dhall, A., Patiyal, S., and Raghava, G.P. (2022). IL13Pred: A method for predicting immunoregulatory cytokine IL-13 inducing peptides. *Computers in Biology and Medicine* 143, 105297.
31. Gupta, S., Sharma, N., Naorem, L.D., Jain, S., and Raghava, G.P. (2022). Collection, compilation and analysis of bacterial vaccines. *Computers in Biology and Medicine* 149, 106030.
32. Dhall, A., Patiyal, S., and Raghava, G.P.S. (2022). HLAnCPred: a method for predicting promiscuous non-classical HLA binding sites. *Brief Bioinform.* 23, bbac192.
33. Bajiya, N., Dhall, A., Aggarwal, S., and Raghava, G.P. (2022). Advances in the field of phage-based therapy with special emphasis on computational resources. *Briefings in Bioinformatics* 23, bbac574.
34. Arora, C., Kaur, D., and Raghava, G.P. (2022). Universal and cross-cancer prognostic biomarkers for predicting survival risk of cancer patients from expression profile of apoptotic pathway genes. *Proteomics* 22, e2000311.
35. Sharma, N., Patiyal, S., Dhall, A., Pande, A., Arora, C., and Raghava, G.P. (2021). AlgPred 2.0: an improved method for predicting allergenic proteins and mapping of IgE epitopes. *Briefings in Bioinformatics* 22, bbaa294.
36. Sharma, N., Patiyal, S., Dhal, A., Devi, N.L., and Raghava, G.P. (2021). ChAIPred: A web server for prediction of allergenicity of chemical compounds. *Comput Biol Med.* 136, 104746.
37. Mathur, D., Kaur, H., Dhall, A., Sharma, N., and Raghava, G.P. (2021). SAPdb: A database of short peptides and the corresponding nanostructures formed by self-assembly. *Computers in Biology and Medicine* 133, 104391.
38. Maryam, L., Usmani, S.S., and Raghava, G.P. (2021). Computational resources in the management of antibiotic resistance: Speeding up drug discovery. *Drug Discovery Today* 26, 2138-2151.
39. Lathwal, A., Kumar, R., and Raghava, G.P. (2021). In-silico identification of subunit vaccine candidates against lung cancer-associated oncogenic viruses. *Computers in Biology and Medicine* 130, 104215.
40. Kumar, V., Patiyal, S., Kumar, R., Sahai, S., Kaur, D., Lathwal, A., and Raghava, G.P. (2021). B3Pdb: An archive of blood-brain barrier-penetrating peptides. *Brain Structure and Function* 226, 2489-2495.
41. Kumar, V., Patiyal, S., Dhall, A., Sharma, N., and Raghava, G.P.S. (2021). B3pred: A random-forest-based method for predicting and designing blood-brain barrier penetrating peptides. *Pharmaceutics* 13, 1237.
42. Kaur, H., Kumar, R., Lathwal, A., and Raghava, G.P. (2021). Computational resources for identification of cancer biomarkers from omics data. *Briefings in functional genomics* 20, 213-222.
43. Kaur, D., Patiyal, S., Arora, C., Singh, R., Lodhi, G., and Raghava, G.P. (2021). In-silico tool for predicting, scanning, and designing Defensins. *Frontiers in Immunology*, 4817.
44. Kaur, D., Arora, C., and Raghava, G.P.S. (2021). Prognostic biomarker-based identification of drugs for managing the treatment of endometrial cancer. *Molecular Diagnosis & Therapy* 25, 629-646.
45. Dwivedi, V.D., Arya, A., Yadav, P., Kumar, R., Kumar, V., and Raghava, G.P. (2021). DenvInD: dengue virus inhibitors database for clinical and molecular research. *Briefings in Bioinformatics* 22, bbaa098.
46. Dhall, A., Patiyal, S., Sharma, N., Usmani, S.S., and Raghava, G.P. (2021). Computer-aided prediction and design of IL-6 inducing peptides: IL-6 plays a crucial role in COVID-19. *Briefings in bioinformatics* 22, 936-945.
47. Dhall, A., Patiyal, S., Sharma, N., Devi, N.L., and Raghava, G.P. (2021). Computer-aided prediction of inhibitors against STAT3 for managing COVID-19. *Comput Biol Med.* 137, 104780.
48. Dhall, A., Jain, S., Sharma, N., Naorem, L.D., Kaur, D., Patiyal, S., and Raghava, G.P. (2021). In silico tools and databases for designing cancer immunotherapy. *Adv Protein Chem Struct Biol.* 129, 1-50.
49. Chaudhary, A., Bhalla, S., Patiyal, S., Raghava, G.P., and Sahni, G. (2021). FermFooDb: A database of bioactive peptides derived from fermented foods. *Helion* 7, e06668.
50. Arora, C., Kaur, D., Naorem, L.D., and Raghava, G.P. (2021). Prognostic biomarkers for predicting papillary thyroid carcinoma patients at high risk using nine genes of apoptotic pathway. *PLoS one* 16, e0259534.
51. Usmani, S.S., and Raghava, G.P. (2020). Potential challenges for coronavirus (SARS-CoV-2) vaccines under trial. *Frontiers in Immunology* 11, 561851.

52. Patiyal, S., Agrawal, P., Kumar, V., Dhall, A., Kumar, R., Mishra, G., and Raghava, G.P. (2020). NAGbinder: An approach for identifying N-acetylglucosamine interacting residues of a protein from its primary sequence. **Protein Science** 29, 201-210.

53. Lathwal, A., Kumar, R., and Raghava, G.P. (2020). OvirusTdb: A database of oncolytic viruses for the advancement of therapeutics in cancer. **Virology** 548, 109-116.

54. Lathwal, A., Kumar, R., and Raghava, G.P. (2020). Computer-aided designing of oncolytic viruses for overcoming translational challenges of cancer immunotherapy. **Drug discovery today** 25, 1198-1205.

55. Lathwal, A., Kumar, R., Arora, C., and Raghava, G.P.S. (2020). Identification of prognostic biomarkers for major subtypes of non-small-cell lung cancer using genomic and clinical data. **Journal of Cancer Research and Clinical Oncology** 146, 2743-2752.

56. Kumar, V., Kumar, R., Agrawal, P., Patiyal, S., and Raghava, G.P. (2020). A Method for Predicting Hemolytic Potency of Chemically Modified Peptides From Its Structure. **Frontiers in Pharmacology** 11, 54.

57. Kumar, R., Lathwal, A., Kumar, V., Patiyal, S., Raghav, P., and Raghava, G. (2020). CancerEnD: A database of cancer associated enhancers. **Genomics** 112, 3696.

58. Kaur, H., Dhall, A., Kumar, R., and Raghava, G.P. (2020). Identification of platform-independent diagnostic biomarker panel for hepatocellular carcinoma using large-scale transcriptomics data. **Frontiers in genetics** 10, 1306.

59. Kaur, H., Bhalla, S., Kaur, D., and Raghava, G.P. (2020). CancerLiver: a database of liver cancer gene expression resources and biomarkers. **Database** 2020.

60. Kaur, H., Bhalla, S., Garg, D., Mehta, N., and Raghava, G. (2020). Analysis and prediction of cholangiocarcinoma from transcriptomic profile of patients. **Journal of Hepatology** 73, A023.

61. Kaur, D., Arora, C., and Raghava, G.P. (2020). A hybrid model for predicting pattern recognition receptors using evolutionary information. **Frontiers in Immunology** 11, 71.

62. Dhall, A., Patiyal, S., Kaur, H., Bhalla, S., Arora, C., and Raghava, G.P. (2020). Computing Skin Cutaneous Melanoma Outcome from the HLA-alleles and Clinical Characteristics. **Frontiers in genetics** 11, 221.

63. Bhalla, S., Kaur, H., Kaur, R., Sharma, S., and Raghava, G.P. (2020). Expression based biomarkers and models to classify early and late-stage samples of Papillary Thyroid Carcinoma. **PLoS one** 15, e0231629.

64. Arora, C., Kaur, D., Lathwal, A., and Raghava, G. (2020). Risk prediction in cutaneous melanoma patients from their clinico-pathological features: superiority of clinical data over gene expression data. **Helix** 6, e04811.

65. Agrawal, P., Mishra, G., and Raghava, G.P. (2020). SAMbinder: A Web Server for Predicting S-Adenosyl-L-Methionine Binding Residues of a Protein From Its Amino Acid Sequence. **Frontiers in pharmacology** 10, 1690.

66. Agrawal, P., Bhagat, D., Mahalwal, M., Sharma, N., and Raghava, G. (2020). AntiCP 2.0: an updated model for predicting anticancer peptides. **Brief Bioinform.** 153, doi:10.1093/bib/bbaa1153.

67. Usmani, S.S., Agrawal, P., Sehgal, M., Patel, P.K., and Raghava, G.P. (2019). ImmunoSPdb: an archive of immunosuppressive peptides. **Database** 2019.

68. Raghav, P.K., Kumar, R., Kumar, V., and Raghava, G.P. (2019). Docking-based approach for identification of mutations that disrupt binding between Bcl-2 and Bax proteins: Inducing apoptosis in cancer cells. **Molecular genetics & genomic medicine** 7, e910.

69. Lathwal, A., Arora, C., and Raghava, G.P. (2019). Prediction of risk scores for colorectal cancer patients from the concentration of proteins involved in mitochondrial apoptotic pathway. **PLoS one** 14, e0217527.

70. Kumar, R., Patiyal, S., Kumar, V., Nagpal, G., and Raghava, G.P. (2019). In Silico Analysis of Gene Expression Change Associated with Copy Number of Enhancers in Pancreatic Adenocarcinoma. **International Journal of Molecular Sciences** 20, 3582.

71. Kumar, R., Nagpal, G., Kumar, V., Usmani, S.S., Agrawal, P., and Raghava, G.P. (2019). HumCFS: a database of fragile sites in human chromosomes. **BMC genomics** 19, 1-8.

72. Kaur, H., Bhalla, S., and Raghava, G.P. (2019). Classification of early and late stage liver hepatocellular carcinoma patients from their genomics and epigenomics profiles. **PLoS one** 14, e0221476.

73. Kaur, D., Patiyal, S., Sharma, N., Usmani, S.S., and Raghava, G.P. (2019). PRRDB 2.0: a comprehensive database of pattern-recognition receptors and their ligands. **Database** 2019.

74. Bhalla, S., Kaur, H., Dhall, A., and Raghava, G.P. (2019). Prediction and analysis of skin cancer progression using genomics profiles of patients. **Scientific Reports** 9, 1-16.

75. Akhter, S., Kaur, H., Agrawal, P., and Raghava, G.P. (2019). RareLSD: a manually curated database of lysosomal enzymes associated with rare diseases. **Database** 2019.

76. Agrawal, P., Singh, H., Srivastava, H.K., Singh, S., Kishore, G., and Raghava, G.P. (2019). Benchmarking of different molecular docking methods for protein-peptide docking. **BMC bioinformatics** 19, 105-124.

77. Agrawal, P., Patiyal, S., Kumar, R., Kumar, V., Singh, H., Raghav, P.K., and Raghava, G.P. (2019). ccPDB 2.0: an updated version of datasets created and compiled from Protein Data Bank. **Database** bay142.
78. Agrawal, P., Kumar, S., Singh, A., Raghava, G.P., and Singh, I.K. (2019). NeuroPIpred: a tool to predict, design and scan insect neuropeptides. **Scientific reports** 9, 1-12.
79. Usmani, S.S., Kumar, R., Kumar, V., Singh, S., and Raghava, G.P. (2018). AntiTbPdb: a knowledgebase of anti-tubercular peptides. **Database** bay025.
80. Usmani, S.S., Kumar, R., Bhalla, S., Kumar, V., and Raghava, G.P. (2018). In Silico Tools and Databases for Designing Peptide-Based Vaccine and Drugs. **Adv Protein Chem Struct Biol.** 112:221-263.
81. Usmani, S.S., Bhalla, S., and Raghava, G.P. (2018). Prediction of antitubercular peptides from sequence information using ensemble classifier and hybrid features. **Frontiers in Pharmacology** 9, 954.
82. Nagpal, G., Usmani, S.S., and Raghava, G.P. (2018). A web resource for designing subunit vaccine against major pathogenic species of bacteria. **Frontiers in immunology** 9, 2280.
83. Nagpal, G., Chaudhary, K., Agrawal, P., and Raghava, G.P. (2018). Computer-aided prediction of antigen presenting cell modulators for designing peptide-based vaccine adjuvants. **Journal of translational medicine** 16, 1-15.
84. Mathur, D., Singh, S., Mehta, A., Agrawal, P., and Raghava, G.P. (2018). In silico approaches for predicting the half-life of natural and modified peptides in blood. **PloS one** 13, e0196829.
85. Mathur, D., Mehta, A., Firmal, P., Bedi, G., Sood, C., Gautam, A., and Raghava, G.P. (2018). TopicalPdb: A database of topically delivered peptides. **Plos one** 13, e0190134.
86. Kumar, V., Agrawal, P., Kumar, R., Bhalla, S., Usmani, S.S., Varshney, G.C., and Raghava, G.P. (2018). Prediction of cell-penetrating potential of modified peptides containing natural and chemically modified residues. **Frontiers in Microbiology** 9, 725.
87. Agrawal, P., and Raghava, G.P. (2018). Prediction of antimicrobial potential of a chemically modified peptide from its tertiary structure. **Frontiers in Microbiology** 9, 2551.
88. Agrawal, P., Raghav, P., Bhalla, S., Sharma, N., and Raghava, G. (2018). Overview of free software developed for designing drugs based on protein-small molecules interaction. **Curr Top Med Chem.** 18(13):1146-1167.
89. Agrawal, P., Bhalla, S., Chaudhary, K., Kumar, R., Sharma, M., and Raghava, G.P. (2018). In silico approach for prediction of antifungal peptides. **Frontiers in Microbiology** 9, 323.
90. Usmani, S.S., Bedi, G., Samuel, J.S., Singh, S., Kalra, S., Kumar, P., Ahuja, A.A., Sharma, M., Gautam, A., and Raghava, G.P. (2017). THPdb: Database of FDA-approved peptide and protein therapeutics. **PloS one** 12, e0181748.
91. Pahil, S., Taneja, N., Ansari, H.R., and Raghava, G. (2017). In silico analysis to identify vaccine candidates common to multiple serotypes of *Shigella* and evaluation of their immunogenicity. **PloS one** 12, e0180505.
92. Nagpal, G., Usmani, S.S., Dhanda, S.K., Kaur, H., Singh, S., Sharma, M., and Raghava, G.P. (2017). Computer-aided designing of immunosuppressive peptides based on IL-10 inducing potential. **Scientific Reports** 7, 42851.
93. Dhanda, S.K., Usmani, S.S., Agrawal, P., Nagpal, G., Gautam, A., and Raghava, G.P. (2017). Novel in silico tools for designing peptide-based subunit vaccines and immunotherapeutics. **Briefings in bioinformatics** 18, 467-478.
94. Bhalla, S., Verma, R., Kaur, H., Kumar, R., Usmani, S.S., Sharma, S., and Raghava, G.P. (2017). CancerPDF: A repository of cancer-associated peptidome found in human biofluids. **Scientific reports** 7, 1511.
95. Bhalla, S., Chaudhary, K., Kumar, R., Sehgal, M., Kaur, H., Sharma, S., and Raghava, G.P. (2017). Gene expression-based biomarkers for discriminating early and late stage of clear cell renal cancer. **Scientific Reports** 7, 44997.
96. Singh, S., Chaudhary, K., Dhanda, S.K., Bhalla, S., Usmani, S.S., Gautam, A., Tuknait, A., Agrawal, P., Mathur, D., and Raghava, G.P. (2016). SATPdb: a database of structurally annotated therapeutic peptides. **Nucleic acids research** 44, D1119-D1126.
97. Singh Nanda, J., Kumar, R., and Raghava, G.P. (2016). dbEM: A database of epigenetic modifiers curated from cancerous and normal genomes. **Scientific reports** 6, 1-6.
98. Singh, H., Srivastava, H.K., and Raghava, G.P. (2016). A web server for analysis, comparison and prediction of protein ligand binding sites. **Biology direct** 11, 14.
99. Singh, H., and Raghava, G.P. (2016). BLAST-based structural annotation of protein residues using Protein Data Bank. **Biology Direct** 11, 1-13.
100. Singh, H., Kumar, R., Singh, S., Chaudhary, K., Gautam, A., and Raghava, G.P. (2016). Prediction of anticancer molecules using hybrid model developed on molecules screened against NCI-60 cancer cell lines. **BMC cancer** 16, 1-10.

101. Mathur, D., Prakash, S., Anand, P., Kaur, H., Agrawal, P., Mehta, A., Kumar, R., Singh, S., and Raghava, G.P. (2016). PEPLife: A Repository of the Half-life of Peptides. **Scientific Reports** 6, 36617.
102. Kumar, R., and Raghava, G.P. (2016). ApoCanD: Database of human apoptotic proteins in the context of cancer. **Scientific Reports** 6, 20797.
103. Gupta, S., Chaudhary, K., Kumar, R., Gautam, A., Nanda, J.S., Dhanda, S.K., Brahmachari, S.K., and Raghava, G.P. (2016). Prioritization of anticancer drugs against a cancer using genomic features of cancer cells: A step towards personalized medicine. **Scientific Reports** 6, 23857.
104. Gupta, S., Chaudhary, K., Dhanda, S.K., Kumar, R., Kumar, S., Sehgal, M., Nagpal, G., and Raghava, G.P. (2016). A platform for designing genome-based personalized immunotherapy or vaccine against cancer. **PloS one** 11, e0166372.
105. Gautam, A., Nanda, J.S., Samuel, J.S., Kumari, M., Priyanka, P., Bedi, G., Nath, S.K., Mittal, G., Khatri, N., and Raghava, G.P.S. (2016). Topical Delivery of Protein and Peptide Using Novel Cell Penetrating Peptide IMT-P8. **Scientific reports** 6, 26278.
106. Dhanda, S.K., Vir, P., Singla, D., Gupta, S., Kumar, S., and Raghava, G.P. (2016). A web-based platform for designing vaccines against existing and emerging strains of *Mycobacterium tuberculosis*. **PloS one** 11, e0153771.
107. Dhanda, S.K., Chaudhary, K., Gupta, S., Brahmachari, S.K., and Raghava, G.P. (2016). A web-based resource for designing therapeutics against Ebola Virus. **Scientific Reports** 6, 24782.
108. Chaudhary, K., Nagpal, G., Dhanda, S.K., and Raghava, G.P. (2016). Prediction of Immunomodulatory potential of an RNA sequence for designing non-toxic siRNAs and RNA-based vaccine adjuvants. **Scientific Reports** 6, 20678.
109. Chaudhary, K., Kumar, R., Singh, S., Tuknait, A., Gautam, A., Mathur, D., Anand, P., Varshney, G.C., and Raghava, G.P. (2016). A Web Server and Mobile App for Computing Hemolytic Potency of Peptides. **Scientific Reports** 6, 22843.
110. Agrawal, P., Bhalla, S., Usmani, S.S., Singh, S., Chaudhary, K., Raghava, G.P., and Gautam, A. (2016). CPPsite 2.0: a repository of experimentally validated cell-penetrating peptides. **Nucleic acids research** 44, D1098-D1103.
111. Tyagi, A., Tuknait, A., Anand, P., Gupta, S., Sharma, M., Mathur, D., Joshi, A., Singh, S., Gautam, A., and Raghava, G.P. (2015). CancerPPD: a database of anticancer peptides and proteins. **Nucleic acids research** 43, D837-D843.
112. Singh, S., Singh, H., Tuknait, A., Chaudhary, K., Singh, B., Kumaran, S., and Raghava, G.P. (2015). PEPstrMOD: structure prediction of peptides containing natural, non-natural and modified residues. **Biology Direct** 10, 1-19.
113. Singh, H., Singh, S., Singla, D., Agarwal, S.M., and Raghava, G.P. (2015). QSAR based model for discriminating EGFR inhibitors and non-inhibitors using Random forest. **Biology direct** 10, 10.
114. Singh, H., Singh, S., and Raghava, G.P. (2015). In silico platform for predicting and initiating  $\beta$ -turns in a protein at desired locations. **Proteins: Structure, Function, and Bioinformatics** 83, 910-921.
115. Panwar, B., and Raghava, G.P. (2015). Identification of protein-interacting nucleotides in a RNA sequence using composition profile of tri-nucleotides. **Genomics** 105, 197-203.
116. Nagpal, G., Gupta, S., Chaudhary, K., Kumar Dhanda, S., Prakash, S., and Raghava, G.P. (2015). VaccineDA: Prediction, design and genome-wide screening of oligodeoxynucleotide-based vaccine adjuvants. **Scientific reports** 5, 1-9.
117. Kumar, R., Singh Chauhan, J., and Pal Singh Raghava, G. (2015). In Silico Designing and Screening of Antagonists against Cancer Drug Target XIAP. **Current cancer drug targets** 15, 836-846.
118. Kumar, R., Chaudhary, K., Singh Chauhan, J., Nagpal, G., Kumar, R., Sharma, M., and Raghava, G.P. (2015). An in silico platform for predicting, screening and designing of antihypertensive peptides. **Scientific reports** 5, 1-10.
119. Kumar, R., Chaudhary, K., Sharma, M., Nagpal, G., Chauhan, J.S., Singh, S., Gautam, A., and Raghava, G.P. (2015). AHTPDB: a comprehensive platform for analysis and presentation of antihypertensive peptides. **Nucleic acids research** 43, D956-D962.
120. Gautam, A., Sharma, M., Vir, P., Chaudhary, K., Kapoor, P., Kumar, R., Nath, S.K., and Raghava, G.P. (2015). Identification and characterization of novel protein-derived arginine-rich cell-penetrating peptides. **European Journal of Pharmaceutics and Biopharmaceutics** 89, 93-106.
121. Dhar, J., Chakrabarti, P., Saini, H., Raghava, G.P.S., and Kishore, R. (2015).  $\omega$ -Turn: A novel  $\beta$ -turn mimic in globular proteins stabilized by main-chain to side-chain C $\equiv$  H $\cdots$  O interaction. **Proteins: Structure, Function, and Bioinformatics** 83, 203-214.

122. Singh, H., Singh, S., and Raghava, G.P. (2014). Evaluation of Protein Dihedral Angle Prediction Methods. **PloS one** 9, e105667.
123. Sharma, A., Singla, D., Rashid, M., and Raghava, G.P. (2014). Designing of peptides with desired half-life in intestine-like environment. **BMC bioinformatics** 15, 282.
124. Panwar, B., and Raghava, G.P. (2014). Prediction of uridine modifications in tRNA sequences. **BMC bioinformatics** 15, 326.
125. Panwar, B., Arora, A., and Raghava, G.P. (2014). Prediction and classification of ncRNAs using structural information. **BMC genomics** 15, 127.
126. Nagpal, G., Sharma, M., Kumar, S., Chaudhary, K., Gupta, S., Gautam, A., and Raghava, G.P. (2014). PCMdb: pancreatic cancer methylation database. **Scientific reports** 4, 4197.
127. Mehta, D., Anand, P., Kumar, V., Joshi, A., Mathur, D., Singh, S., Tuknait, A., Chaudhary, K., Gautam, S.K., and Gautam, A. (2014). ParaPep: a web resource for experimentally validated antiparasitic peptide sequences and their structures. **Database** 2014, bau051.
128. Kumar, R., Chaudhary, K., Singla, D., Gautam, A., and Raghava, G.P. (2014). Designing of promiscuous inhibitors against pancreatic cancer cell lines. **Scientific reports** 4, 4668.
129. Gautam, A., Kapoor, P., Chaudhary, K., Kumar, R., Raghava, G., and Consortium, S.D.D. (2014). Tumor Homing Peptides as Molecular Probes for Cancer Therapeutics, Diagnostics and Theranostics. **Current medicinal chemistry** 21, 2367-2391.
130. Chauhan, J.S., Dhanda, S.K., Singla, D., Agarwal, S.M., Raghava, G.P., and Consortium, O.S.D.D. (2014). QSAR-Based Models for Designing Quinazoline/ Imidazothiazoles/ Pyrazolopyrimidines Based Inhibitors against Wild and Mutant EGFR. **PLOS ONE** 9, e101079.
131. Ahmad, S., Gupta, S., Kumar, R., Varshney, G.C., and Raghava, G.P. (2014). Herceptin resistance database for understanding mechanism of resistance in breast cancer patients. **Scientific reports** 4, 4483.
132. Vikram, S., Pandey, J., Kumar, S., and Raghava, G.P.S. (2013). Genes Involved in Degradation of para-Nitrophenol Are Differentially Arranged in Form of Non-Contiguous Gene Clusters in *Burkholderia* sp. strain SJ98. **PloS one** 8, e84766.
133. Tyagi, A., Kapoor, P., Kumar, R., Chaudhary, K., Gautam, A., and Raghava, G. (2013). In silico models for designing and discovering novel anticancer peptides. **Scientific reports** 3, 1-8.
134. Singla, D., Tewari, R., Kumar, A., and Raghava, G.P. (2013). Designing of inhibitors against drug tolerant *Mycobacterium tuberculosis* (H37Rv). **Chemistry Central Journal** 7, 49.
135. Singla, D., Dhanda, S.K., Chauhan, J.S., Bhardwaj, A., Brahmachari, S.K., and Raghava, G.P. (2013). Open Source Software and Web Services for Designing Therapeutic Molecules. **Current topics in medicinal chemistry** 13, 1172-1191.
136. Singh, H., Ansari, H.R., and Raghava, G.P. (2013). Improved method for linear B-cell epitope prediction using Antigen's primary sequence. **PloS one** 8, e62216.
137. Sharma, A., Kapoor, P., Gautam, A., Chaudhary, K., Kumar, R., Chauhan, J.S., Tyagi, A., and Raghava, G.P. (2013). Computational approach for designing tumor homing peptides. **Scientific reports** 3, 1607.
138. Panwar, B., Gupta, S., and Raghava, G.P. (2013). Prediction of vitamin interacting residues in a vitamin binding protein using evolutionary information. **BMC bioinformatics** 14, 44.
139. Mangal et al. (2013). NPACT: naturally occurring plant-based anti-cancer compound-activity-target database. **Nucleic acids research** 41, D1124-D1129.
140. Kumar, S., Vikram, S., and Raghava, G.P.S. (2013). Genome annotation of *Burkholderia* sp. SJ98 with special focus on chemotaxis genes. **PloS one** 8, e70624.
141. Kumar, R., Raghava, G.P., and Abrams, W.R. (2013). Hybrid approach for predicting coreceptor used by HIV-1 from its V3 loop amino acid sequence. **PloS one** 8.
142. Kumar, R., Chaudhary, K., Gupta, S., Singh, H., Kumar, S., Gautam, A., Kapoor, P., and Raghava, G.P. (2013). CancerDR: cancer drug resistance database. **Scientific reports** 3, 1445.
143. Gupta, S., Kapoor, P., Chaudhary, K., Gautam, A., Kumar, R., Raghava, G.P., and Consortium, O.S.D.D. (2013). In Silico Approach for Predicting Toxicity of Peptides and Proteins. **PloS one** 8, e73957.
144. Gupta, S., Ansari, H.R., Gautam, A., Raghava, G., and Consortium, O.S.D.D. (2013). Identification of B-cell epitopes in an antigen for inducing specific class of antibodies. **Biology direct** 8, 27.
145. Gautam, A., Chaudhary, K., Singh, S., Joshi, A., Anand, P., Tuknait, A., Mathur, D., Varshney, G.C., and Raghava, G.P. (2013). Hemolytik: a database of experimentally determined hemolytic and non-hemolytic peptides. **Nucleic acids research**, gkt1008.
146. Gautam, A., Chaudhary, K., Kumar, R., Sharma, A., Kapoor, P., Tyagi, A., and Raghava, G. (2013). In silico approaches for designing highly effective cell penetrating peptides. **J Transl Med** 11, 74.

147. Dhanda, S.K., Vir, P., and Raghava, G.P. (2013). Designing of interferon-gamma inducing MHC class-II binders. **Biology direct** 8, 1-15.

148. Dhanda, S.K., Singla, D., Mondal, A.K., and Raghava, G.P. (2013). DrugMint: a webserver for predicting and designing of drug-like molecules. **Biology direct** 8, 1-12.

149. Dhanda, S.K., Gupta, S., Vir, P., and Raghava, G. (2013). Prediction of IL4 inducing peptides. **Clinical and Developmental Immunology** 2013.

150. Chauhan, J.S., Rao, A., and Raghava, G.P. (2013). In silico platform for prediction of N-, O-and C-glycosites in eukaryotic protein sequences. **PLoS one** 8, e67008.

151. Ahmed, F., Kaundal, R., and Raghava, G.P. (2013). PHDcleav: a SVM based method for predicting human Dicer cleavage sites using sequence and secondary structure of miRNA precursors. **BMC bioinformatics** 14, S9.

152. Singh, H., Chauhan, J.S., Gromiha, M.M., and Raghava, G.P. (2012). ccPDB: compilation and creation of data sets from Protein Data Bank. **Nucleic Acids Research** 40, D486-D489.

153. Kumar, S., Vikram, S., and Raghava, G.P.S. (2012). Genome sequence of the nitroaromatic compound-degrading bacterium Burkholderia sp. strain SJ98. **Journal of bacteriology** 194, 3286.

154. Kapoor, P., Singh, H., Gautam, A., Chaudhary, K., Kumar, R., and Raghava, G.P. (2012). TumorHoPe: a database of tumor homing peptides. **PLoS One** 7, e35187.

155. Gautam, A., Singh, H., Tyagi, A., Chaudhary, K., Kumar, R., Kapoor, P., and Raghava, G. (2012). CPPsite: a curated database of cell penetrating peptides. **Database** 2012, bas015.

156. Chauhan, J.S., Bhat, A.H., Raghava, G.P., and Rao, A. (2012). GlycoPP: a webserver for prediction of N-and O-glycosites in prokaryotic protein sequences. **PLoS one** 7, e40155.

157. Bhat, A.H., Mondal, H., Chauhan, J.S., Raghava, G.P., Methi, A., and Rao, A. (2012). ProGlycProt: a repository of experimentally characterized prokaryotic glycoproteins. **Nucleic acids research** 40, D388-D393.

158. Aithal, A., Sharma, A., Joshi, S., Raghava, G.P., and Varshney, G.C. (2012). PolysacDB: A Database of Microbial Polysaccharide Antigens and Their Antibodies. **PLoS one** 7, e34613.

159. Singla, D., Anurag, M., Dash, D., and Raghava, G.P. (2011). A web server for predicting inhibitors against bacterial target GlmU protein. **BMC pharmacology** 11, 1-9.

160. Panwar, B., and Raghava, G.P. (2011). Predicting sub-cellular localization of tRNA synthetases from their primary structures. **Amino Acids**, 1-11.

161. Mishra, N.K., and Raghava, G. (2011). Prediction of specificity and cross-reactivity of kinase inhibitors. **Lett Drug Des Discov** 8, 223-228.

162. Kumar, R., Panwar, B., Chauhan, J.S., and Raghava, G.P. (2011). Analysis and prediction of cancerlectins using evolutionary and domain information. **BMC research notes** 4, 237.

163. Kumar, M., Gromiha, M.M., and Raghava, G.P. (2011). SVM based prediction of RNA-binding proteins using binding residues and evolutionary information. **Journal of Molecular Recognition** 24, 303-313.

164. Ahmed, F., and Raghava, G.P. (2011). Designing of Highly Effective Complementary and Mismatch siRNAs for Silencing a Gene. **PLoS ONE** 6, e23443.

165. Agarwal, S., Kumar Mishra, N., Singh, H., and Raghava, G.P. (2011). Identification of mannose interacting residues using local composition. **PLoS one** 6, e24039\_24031-e24039\_24039.

166. Verma, R., Varshney, G.C., and Raghava, G. (2010). Prediction of mitochondrial proteins of malaria parasite using split amino acid composition and PSSM profile. **Amino acids** 39, 101-110.

167. Rashid, M., Ramasamy, S., and Raghava, G. (2010). A Simple Approach for Predicting Protein-Protein Interactions. **Current Protein and Peptide Science** 11, 589-600.

168. Panwar, B., and Raghava, G.P. (2010). Prediction and classification of aminoacyl tRNA synthetases using PROSITE domains. **BMC genomics** 11, 507.

169. Mishra, N.K., and Raghava, G.P. (2010). Prediction of FAD interacting residues in a protein from its primary sequence using evolutionary information. **BMC bioinformatics** 11, S48.

170. Mishra, N.K., Agarwal, S., and Raghava, G.P. (2010). Prediction of cytochrome P450 isoform responsible for metabolizing a drug molecule. **BMC pharmacology** 10, 1-9.

171. Lata, S., Mishra, N.K., and Raghava, G.P. (2010). AntiBP2: improved version of antibacterial peptide prediction. **BMC bioinformatics** 11, S19.

172. Garg, A., Tewari, R., and Raghava, G.P. (2010). Virtual screening of potential drug-like inhibitors against Lysine/DAP pathway of Mycobacterium tuberculosis. **BMC bioinformatics** 11, S53.

173. Garg, A., Tewari, R., and Raghava, G.P. (2010). KiDoQ: using docking based energy scores to develop ligand based model for predicting antibacterials. **BMC bioinformatics** 11, 125.

174. Chauhan, J.S., Mishra, N.K., and Raghava, G.P. (2010). Prediction of GTP interacting residues, dipeptides and tripeptides in a protein from its evolutionary information. **BMC bioinformatics** 11, 301.

175. Ansari, H.R., and Raghava, G.P. (2010). Identification of conformational B-cell Epitopes in an antigen from its primary sequence. *Immunome research* 6, 1-9.

176. Ansari, H.R., and Raghava, G.P. (2010). Identification of NAD interacting residues in proteins. *BMC bioinformatics* 11, 160.

177. Ansari, H.R., Flower, D.R., and Raghava, G. (2010). AntigenDB: an immunoinformatics database of pathogen antigens. *Nucleic acids research* 38, D847-D853.

178. Agarwal, S.M., Raghav, D., Singh, H., and Raghava, G. (2010). CCDB: a curated database of genes involved in cervix cancer. *Nucleic acids research* 39, D975-D979.

179. Rashid, M., Singla, D., Sharma, A., Kumar, M., and Raghava, G.P. (2009). Hmrbase: a database of hormones and their receptors. *BMC genomics* 10, 307.

180. Lata, S., and Raghava, G. (2009). Prediction and classification of chemokines and their receptors. *Protein Engineering Design and Selection*, gzp016.

181. Kumar, M., and Raghava, G.P. (2009). Prediction of nuclear proteins using SVM and HMM models. *BMC bioinformatics* 10, 22.

182. Kaundal, R., and Raghava, G.P. (2009). RSLpred: an integrative system for predicting subcellular localization of rice proteins combining compositional and evolutionary information. *Proteomics* 9, 2324-2342.

183. Chauhan, J.S., Mishra, N.K., and Raghava, G.P. (2009). Identification of ATP binding residues of a protein from its primary sequence. *BMC bioinformatics* 10, 434.

184. Ahmed, F., Kumar, M., and Raghava, G.P. (2009). Prediction of polyadenylation signals in human DNA sequences using nucleotide frequencies. *In silico biology* 9, 135-148.

185. Ahmed, F., Ansari, H.R., and Raghava, G.P. (2009). Prediction of guide strand of microRNAs from its sequence and secondary structure. *BMC bioinformatics* 10, 105.

186. Verma, R., Tiwari, A., Kaur, S., Varshney, G.C., and Raghava, G.P. (2008). Identification of Proteins Secreted by Malaria Parasite into Erythrocyte using SVM and PSSM profiles. *BMC bioinformatics* 9, 201.

187. Sethi, D., Garg, A., and Raghava, G. (2008). DPROT: prediction of disordered proteins using evolutionary information. *Amino Acids* 35, 599-605.

188. Lata, S., and Raghava, G.P. (2008). PRRDB: a comprehensive database of pattern-recognition receptors and their ligands. *BMC genomics* 9, 180.

189. Lata, S., and Raghava, G. (2008). CytoPred: a server for prediction and classification of cytokines. *Protein Engineering, Design & Selection* 21, 279-282.

190. Kumar, M., Thakur, V., and Raghava, G.P. (2008). COPid: composition based protein identification. *In silico biology* 8, 121-128.

191. Kumar, M., Gromiha, M.M., and Raghava, G. (2008). Prediction of RNA binding sites in a protein using SVM and PSSM profile. *Proteins: Structure, Function, and Bioinformatics* 71, 189-194.

192. Garg, A., and Raghava, G.P. (2008). ESLpred2: improved method for predicting subcellular localization of eukaryotic proteins. *BMC bioinformatics* 9, 503.

193. Garg, A., and Raghava, G.P. (2008). A machine learning based method for the prediction of secretory proteins using amino acid composition, their order and similarity-search. *In silico biology* 8, 129-140.

194. Saha, S., and Raghava, G.P. (2007). BTXpred: prediction of bacterial toxins. *In silico biology* 7, 405-412.

195. Saha, S., and Raghava, G.P. (2007). Prediction of neurotoxins based on their function and source. *In silico biology* 7, 369-387.

196. Rashid, M., Saha, S., and Raghava, G.P. (2007). Support Vector Machine-based method for predicting subcellular localization of mycobacterial proteins using evolutionary information and motifs. *BMC bioinformatics* 8, 1-9.

197. Muthukrishnan, S., Garg, A., and Raghava, G. (2007). Oxypred: prediction and classification of oxygen-binding proteins. *Genomics, proteomics & bioinformatics* 5, 250-252.

198. Mishra, N.K., Kumar, M., and Raghava, G. (2007). Support vector machine based prediction of glutathione S-transferase proteins. *Protein and peptide letters* 14, 575-580.

199. Lata, S., Sharma, B., and Raghava, G. (2007). Analysis and prediction of antibacterial peptides. *BMC bioinformatics* 8, 1-10.

200. Kaur, H., Garg, A., and Raghava, G. (2007). PEPstr: a de novo method for tertiary structure prediction of small bioactive peptides. *Protein and peptide letters* 14, 626-631.

201. Bhasin, M., and Raghava, G. (2007). A hybrid approach for predicting promiscuous MHC class I restricted T cell epitopes. *Journal of biosciences* 32, 31-42.

202. Singh, M.K., Srivastava, S., Raghava, G., and Varshney, G.C. (2006). HaptenDB: a comprehensive database of haptens, carrier proteins and anti-hapten antibodies. *Bioinformatics* 22, 253-255.

203. Saha, S., Zack, J., Singh, B., and Raghava, G. (2006). VGchan: prediction and classification of voltage-gated ion channels. **Genomics, proteomics & bioinformatics** 4, 253-258.

204. Saha, S., and Raghava, G. (2006). VICMpred: an SVM-based method for the prediction of functional proteins of Gram-negative bacteria using amino acid patterns and composition. **Genomics, proteomics & bioinformatics** 4, 42-47.

205. Saha, S., and Raghava, G. (2006). AlgPred: prediction of allergenic proteins and mapping of IgE epitopes. **Nucleic acids research** 34, W202-W209.

206. Saha, S., and Raghava, G. (2006). Prediction of continuous B-cell epitopes in an antigen using recurrent neural network. **Proteins: Structure, Function, and Bioinformatics** 65, 40-48.

207. Kumar, M., Verma, R., and Raghava, G.P. (2006). Prediction of mitochondrial proteins using support vector machine and hidden Markov model. **Journal of Biological Chemistry** 281, 5357-5363.

208. Kaur, H., and Raghava, G.P. (2006). Prediction of  $\text{Ca-H}\cdot\text{O}$  and  $\text{Ca-H}\cdot\pi$  Interactions in Proteins Using Recurrent Neural Network. **In silico biology** 6, 111-125.

209. Kaundal, R., Kapoor, A.S., and Raghava, G.P. (2006). Machine learning techniques in disease forecasting: a case study on rice blast prediction. **BMC bioinformatics** 7, 485.

210. Saha, S., Bhasin, M., and Raghava, G.P. (2005). Bcipep: a database of B-cell epitopes. **BMC genomics** 6, 1-7.

211. Kumar, M., Bhasin, M., Natt, N.K., and Raghava, G. (2005). BhairPred: prediction of  $\beta$ -hairpins in a protein from multiple alignment information using ANN and SVM techniques. **Nucleic acids research** 33, W154-W159.

212. Garg, A., Kaur, H., and Raghava, G. (2005). Real value prediction of solvent accessibility in proteins using multiple sequence alignment and secondary structure. **Proteins: Structure, Function, and Bioinformatics** 61, 318-324.

213. Garg, A., Bhasin, M., and Raghava, G.P. (2005). Support vector machine-based method for subcellular localization of human proteins using amino acid compositions, their order, and similarity search. **Journal of Biological Chemistry** 280, 14427-14432.

214. Bhasin, M., and Raghava, G. (2005). GPCRsclass: a web tool for the classification of amine type of G-protein-coupled receptors. **Nucleic acids research** 33, W143-W147.

215. Bhasin, M., and Raghava, G. (2005). Pcleavage: an SVM based method for prediction of constitutive proteasome and immunoproteasome cleavage sites in antigenic sequences. **Nucleic acids research** 33, W202-W207.

216. Bhasin, M., Garg, A., and Raghava, G. (2005). PSLpred: prediction of subcellular localization of bacterial proteins. **Bioinformatics** 21, 2522-2524.

217. Natt, N.K., Kaur, H., and Raghava, G. (2004). Prediction of transmembrane regions of  $\beta$ -barrel proteins using ANN-and SVM-based methods. **PROTEINS: Structure, Function, and Bioinformatics** 56, 11-18.

218. Kaur, H., and Raghava, G.P.S. (2004). Prediction of  $\beta$ -turns in proteins from multiple alignment using neural network. **Protein Science** 12, 627-634.

219. Kaur, H., and Raghava, G. (2004). Role of evolutionary information in prediction of aromatic-backbone NH interactions in proteins. **FEBS letters** 564, 47-57.

220. Kaur, H., and Raghava, G. (2004). Prediction of  $\alpha$ -turns in proteins using PSI-BLAST profiles and secondary structure information. **Proteins: Structure, Function, and Bioinformatics** 55, 83-90.

221. Kaur, H., and Raghava, G. (2004). A neural network method for prediction of  $\beta$ -turn types in proteins using evolutionary information. **Bioinformatics** 20, 2751-2758.

222. Issac, B., and Raghava, G.P.S. (2004). EGPred: prediction of eukaryotic genes using ab initio methods after combining with sequence similarity approaches. **Genome research** 14, 1756-1766.

223. Bhasin, M., and Raghava, G.P. (2004). Classification of nuclear receptors based on amino acid composition and dipeptide composition. **Journal of Biological Chemistry** 279, 23262-23266.

224. Bhasin, M., and Raghava, G. (2004). Analysis and prediction of affinity of TAP binding peptides using cascade SVM. **Protein Science** 13, 596-607.

225. Bhasin, M., and Raghava, G. (2004). GPCRpred: an SVM-based method for prediction of families and subfamilies of G-protein coupled receptors. **Nucleic acids research** 32, W383-W389.

226. Bhasin, M., and Raghava, G. (2004). SVM based method for predicting HLA-DRB1\* 0401 binding peptides in an antigen sequence. **Bioinformatics** 20, 421-423.

227. Bhasin, M., and Raghava, G. (2004). Prediction of CTL epitopes using QM, SVM and ANN techniques. **Vaccine** 22, 3195-3204.

228. Bhasin, M., and Raghava, G. (2004). ESLpred: SVM-based method for subcellular localization of eukaryotic proteins using dipeptide composition and PSI-BLAST. **Nucleic acids research** 32, W414-W419.

229. Singh, H., and Raghava, G. (2003). ProPred1: prediction of promiscuous MHC Class-I binding sites. *Bioinformatics* 19, 1009-1014.
230. Kaur, H., and Raghava, G. (2003). A neural-network based method for prediction of  $\gamma$ -turns in proteins from multiple sequence alignment. *Protein science* 12, 923-929.
231. Bhasin, M., Singh, H., and Raghava, G. (2003). MHCBN: A Comprehensive Database of MHC Binding and Non-Binding Peptides. *Bioinformatics* 19, 665.
232. Kaur, H., and Raghava, G. (2002). BetaTPred: prediction of  $\beta$ -TURNs in a protein using statistical algorithms. *Bioinformatics* 18, 498-499.
233. Kaur, H., and Raghava, G. (2002). An evaluation of  $\beta$ -turn prediction methods. *Bioinformatics* 18, 1508-1514.
234. Issac, B., Singh, H., Kaur, H., and Raghava, G. (2002). Locating probable genes using Fourier transform approach. *Bioinformatics* 18, 196-197.
235. Issac, B., and Raghava, G. (2002). GWFASTA: server for FASTA search in eukaryotic and microbial genomes. *Biotechniques* 33, 548-556.
236. Singh, H., and Raghava, G. (2001). ProPred: prediction of HLA-DR binding sites. *Bioinformatics* 17, 1236-1237.

## 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.
2. Tomer R, Patiyal S, Kaur D, Choudhury S, Raghava GP (2024) Genome-based solutions for managing mucormycosis. *Adv Protein Chem Struct Biol*. 139:383-403.
3. Jain S, Malhotra KPK, Patiyal S, Raghava GP. (2023) A Highly Accurate Model for Screening Prostate Cancer Using Propensity Index Panel of Ten Genes. *J Comput Biol*. 30(12):1305-1314.
4. Pande et al. (2023). Pfeature: A Tool for Computing Wide Range of Protein Features and Building Prediction Models. *Journal of Computational Biology* 30, 204-222.
5. Sun, D., Nguyen, T.M., Allaway, R.J., Wang, J., Chung, V., Thomas, V.Y., Mason, M., Dimitrovsky, I., Ericson, L., and Li, H. (2022). A Crowdsourcing Approach to Develop Machine Learning Models to Quantify Radiographic Joint Damage in Rheumatoid Arthritis. *JAMA Netw Open*. 5, e2227423.
6. Patiyal, S., Dhall, A., and Raghava, G.P. (2022). Prediction of risk-associated genes and high-risk liver cancer patients from their mutation profile: Benchmarking of mutation calling techniques. *Biology Methods and Protocols* 7, bpac012.
7. Tarca, A.L., Pataki, B.Á., Romero, R., Sirota, M., Guan, Y., Kutum, R., Gomez-Lopez, N., Done, B., Bhatti, G., and Yu, T. (2021). Crowdsourcing assessment of maternal blood multi-omics for predicting gestational age and preterm birth. *Cell Reports Medicine* 2.
8. Sieberts, S.K., Schaff, J., Duda, M., Pataki, B.Á., Sun, M., Snyder, P., Daneault, J.-F., Parisi, F., Costante, G., and Rubin, U. (2021). Crowdsourcing digital health measures to predict Parkinson's disease severity: the Parkinson's Disease Digital Biomarker DREAM Challenge. *npj Digital Medicine* 4, 1-12.
9. Sapra, D., Kaur, H., Dhall, A., and Raghava, G.P. (2021). ProCanBio: a database of manually curated biomarkers for Prostate Cancer. *Journal of Computational Biology* 28, 1248-1257.
10. Gabor A, T.M., Driessen A, Tanevski J, Guo B, Cao W, Shen H, Yu T, Chung V, and Single Cell Signaling in Breast Cancer DREAM Consortium members, B.B., Saez-Rodriguez J (2021). Cell-to-cell and type-to-type heterogeneity of signaling networks: insights from the crowd. *Mol Syst Biol*. 17, e10402.
11. Yang, M., Petralia, F., Li, Z., Li, H., Ma, W., Song, X., Kim, S., Lee, H., Yu, H., and Lee, B. (2020). Community Assessment of the Predictability of Cancer Protein and Phosphoprotein Levels from Genomics and Transcriptomics. *Cell Systems* 11, 186-195. e189.
12. Patiyal, S., Kaur, D., Kaur, H., Sharma, N., Dhall, A., Sahai, S., Agrawal, P., Maryam, L., Arora, C., and Raghava, G.P. (2020). A Web-Based Platform on Coronavirus Disease-19 to Maintain Predicted Diagnostic, Drug, and Vaccine Candidates. *Monoclonal Antibodies in Immunodiagnosis and Immunotherapy* 39, 204-216.
13. Mason, M.J., Schinke, C., Eng, C.L., Towfic, F., Gruber, F., Dervan, A., White, B.S., Pratapa, A., Guan, Y., and Chen, H. (2020). Multiple Myeloma DREAM Challenge reveals epigenetic regulator PHF19 as marker of aggressive disease. *Leukemia* 34, 1866-1874.
14. Brown, P., Tan, A.-C., El-Esawi, M.A., Liehr, T., Blanck, O., Gladue, D.P., Almeida, G.M., Cernava, T., Sorzano, C.O., and Yeung, A.W. (2019). Large expert-curated database for benchmarking document similarity detection in biomedical literature search. *Database* 2019.
15. Ahmad, S., Gromiha, M.M., Raghava, G.P., Schönbach, C., and Ranganathan, S. (2019). APBioNet's annual International Conference on Bioinformatics (InCoB) returns to India in 2018. *BioMed Central*.
16. Kumar, R., Kaur, R., Bhondekar, A.P., and Raghava, G.P. (2018). Human Opinion Inspired Feature Selection Strategy for Predicting the Pleasantness of a Molecule. *Advances in Intelligent Systems and Computing*, 706:197-205.
17. Keller, A., Gerkin, R.C., Guan, Y., Dhurandhar, A., Turu, G., Szalai, B., Mainland, J.D., Ihara, Y., Yu, C.W., and Wolfinger, R. (2017). Predicting human olfactory perception from chemical features of odor molecules. *Science*, eaal2014.
18. Gaur, A., Bhardwaj, A., Sharma, A., John, L., Vivek, M., Tripathi, N., Bharatam, P., Kumar, R., Janardhan, S., and Mori, A. (2017). Assessing therapeutic potential of molecules: molecular property diagnostic suite for tuberculosis. *J Chem Sci* 129, 515–531.
19. Bhalla, S., Sharma, S., and Raghava, G.P.S. (2017). Challenges in Prediction of different Cancer Stages using Gene Expression Profile of Cancer Patients. *ACM* pp. 602-602.

20. Bairdara, P., Gautam, A., Raghava, G., and Korpole, S. (2017). Anticancer properties of a defensin like class II bacteriocin Laterosporulin10. **Scientific reports** 7, 46541.
21. Randhawa, H.K., Gautam, A., Sharma, M., Bhatia, R., Varshney, G.C., Raghava, G.P.S., and Nandanwar, H. (2016). Cell-penetrating peptide and antibiotic combination therapy: a potential alternative to combat drug resistance in methicillin-resistant *Staphylococcus aureus*. **Applied microbiology and biotechnology** 100, 4073-4083.
22. Nupur, L., Vats, A., Dhanda, S.K., Raghava, G.P., Pinnaka, A.K., and Kumar, A. (2016). ProCarDB: a database of bacterial carotenoids. **BMC microbiology** 16, 1-8.
23. Kumar, R., Kaur, R., Bhondekar, A.P., and Raghava, G.P.S. (2016). Smell and language: datacentric approach to predicting smell of a molecule. **Journal of Digital Olfaction Society** 4.
24. Gupta, et al. (2016). ZikaVR: An Integrated Zika Virus Resource for Genomics, Proteomics, Phylogenetic and Therapeutic Analysis. **Scientific Reports** 6, 32713.
25. Bhatia, R., Gautam, A., Gautam, S.K., Mehta, D., Kumar, V., Raghava, G.P., and Varshney, G.C. (2015). Assessment of SYBR green I dye-based fluorescence assay for screening antimalarial activity of cationic peptides and DNA intercalating agents. **Antimicrobial agents and chemotherapy** 59, 2886-2889.
26. S Yadav, I., Singh, H., Khan, I., Chaudhury, A., Raghava, G., and M Agarwal, S. (2014). EGFRIndb: Epidermal Growth Factor Receptor Inhibitor Database. **Anti-Cancer Agents in Medicinal Chemistry** 14, 928-935.
27. Mishra, N.K., Singla, D., Agarwal, S., and Raghava, G.P.S. (2014). ToxiPred: A Server for Prediction of Aqueous Toxicity of Small Chemical Molecules in *T. Pyriformis*. **Journal of Translational Toxicology** 1, 21-27.
28. Vikram, S., Kumar, S., Vaidya, B., Pinnaka, A.K., and Raghava, G.P.S. (2013). Draft genome sequence of the 2-chloro-4-nitrophenol-degrading bacterium *Arthrobacter* sp. strain SJCon. **Genome announcements** 1, e00058-00013.
29. Singh SV, Kumar N, Singh SN, Bhattacharya T, Sohal JS, Singh PK, Singh AV, Singh B, Chaubey KK, Gupta S, Sharma N, Kumar S, Raghava GP. (2013). Genome sequence of the “Indian Bison Type” biotype of *Mycobacterium avium* subsp. *paratuberculosis* strain S5. **Genome announcements** 1, e00005-00013.
30. Singh, N.K., Kumar, S., Raghava, G.P.S., and Mayilraj, S. (2013). Draft genome sequence of *Acinetobacter baumannii* strain MSP4-16. **Genome announcements** 1, e00137-00113.
31. Kumar, S., Kaur, N., Singh, N.K., Raghava, G.P.S., and Mayilraj, S. (2013). Draft genome sequence of *Streptomyces ganicidicus* strain BKS 13-15. **Genome announcements** 1, e00150-00113.
32. Kumar, S., Kaur, C., Kimura, K., Takeo, M., Raghava, G.P.S., and Mayilraj, S. (2013). Draft genome sequence of the type species of the genus *Citrobacter*, *Citrobacter freundii* MTCC 1658. **Genome announcements** 1, e00120-00112.
33. Kumar, S., Kaur, C., Kimura, K., Takeo, M., Raghava, G., and Mayilraj, S. (2013). Draft genome sequence of the type species of the genus *Citrobacter*, *Citrobacter freundii* MTCC 1658. **Genome Announc** 1 (1): e00120-12.
34. Kumar, S., Bala, M., Raghava, G.P.S., and Mayilraj, S. (2013). Draft genome sequence of *Rhodococcus triatomae* strain BKS 15-14. **Genome announcements** 1, e00129-00113.
35. Kaur, N., Kumar, S., Bala, M., Raghava, G.P.S., and Mayilraj, S. (2013). Draft genome sequence of *Amycolatopsis decaplanina* strain DSM 44594T. **Genome announcements** 1, e00138-00113.
36. Bhartiya, D., Pal, K., Ghosh, S., Kapoor, S., Jalali, S., Panwar, B., Jain, S., Sati, S., Sengupta, S., and Sachidanandan, C. (2013). IncRNome: a comprehensive knowledgebase of human long noncoding RNAs. **Database** 2013, bat034.
37. Bala, M., Kumar, S., Raghava, G.P.S., and Mayilraj, S. (2013). Draft genome sequence of *Rhodococcus ruber* strain BKS 20-38. **Genome announcements** 1, e00139-00113.
38. Bala, M., Kumar, S., Raghava, G.P.S., and Mayilraj, S. (2013). Draft genome sequence of *Rhodococcus qingshengii* strain BKS 20-40. **Genome announcements** 1, e00128-00113.
39. Vikram, S., Pandey, J., Bhalla, N., Pandey, G., Ghosh, A., Khan, F., Jain, R.K., and Raghava, G.P. (2012). Branching of the p-nitrophenol (PNP) degradation pathway in *burkholderia* sp. Strain SJ98: Evidences from genetic characterization of PNP gene cluster. **AMB Express** 2, 1-10.
40. Vikram, S., Kumar, S., Subramanian, S., and Raghava, G.P.S. (2012). Draft genome sequence of the nitrophenol-degrading actinomycete *Rhodococcus imtechensis* RKJ300. **American Society for Microbiology** 1752 N St., NW, Washington, DC.
41. Kumar, S., Vikram, S., Subramanian, S., Raghava, G.P.S., and Pinnaka, A.K. (2012). Genome Sequence of the Halotolerant Bacterium *Imtechella halotolerans* K1T. **Journal of bacteriology** 194, 3731.
42. Kumar, S., Subramanian, S., Raghava, G.P.S., and Pinnaka, A.K. (2012). Genome sequence of the marine bacterium *Marinilabilia salmonicolor* JCM 21150T. **Journal of bacteriology** 194, 3746.

43. Kumar, S., Randhawa, A., Ganesan, K., Raghava, G.P.S., and Mondal, A.K. (2012). Draft genome sequence of salt-tolerant yeast *Debaryomyces hansenii* var. *hansenii* MTCC 234. **American Society for Microbiology** 1752 N St., NW, Washington, DC.
44. Kumar, S., Kushwaha, H., Bachhawat, A.K., Raghava, G.P.S., and Ganesan, K. (2012). Genome sequence of the oleaginous red yeast *Rhodosporidium toruloides* MTCC 457. **American Society for Microbiology** 1752 N St., NW, Washington, DC.
45. Zhang, G.L., Ansari, H.R., Bradley, P., Cawley, G.C., Hertz, T., Hu, X., Jovic, N., Kim, Y., Kohlbacher, O., and Lund, O. (2011). Machine learning competition in immunology—Prediction of HLA class I binding peptides. **Journal of immunological methods** 374, 1-4.
46. Tyagi, A., Ahmed, F., Thakur, N., Sharma, A., Raghava, G.P., and Kumar, M. (2011). HIVsirDB: a database of HIV inhibiting siRNAs. **PLoS One** 6, e25917\_25911-e25917\_25916.
47. Kumar Mishra, N., and Raghava, P. (2011). Prediction of Specificity and Cross-Reactivity of Kinase Inhibitors. **Letters in Drug Design & Discovery** 8, 223-228.
48. Bhardwaj, A., Scaria, V., Raghava, G.P.S., Lynn, A.M., Chandra, N., Banerjee, S., Raghunandanan, M.V., Pandey, V., Taneja, B., and Yadav, J. (2011). Open source drug discovery—A new paradigm of collaborative research in tuberculosis drug development. **Tuberculosis** 91, 479-486.
49. Singla, D., Sharma, A., Kaur, J., Panwar, B., and Raghava, G.P. (2010). BIAdb: a curated database of benzylisoquinoline alkaloids. **BMC pharmacology** 10, 1-8.
50. Anastas, P., Bejatolah, M.-K., and Gajendra, P. (2010). Bridging Innate and Adaptive Antitumor Immunity Targeting Glycans. **Journal of Biomedicine and Biotechnology** 2010.
51. Raghava, G.P.S. (2009). Is citation a good criterion? **Nature India** 133.
52. Lata, S., Bhasin, M., and Raghava, G.P. (2009). MHCBN 4.0: A database of MHC/TAP binding peptides and T-cell epitopes. **BMC research notes** 2, 61.
53. Chaudhary, N., Mahajan, L., Madan, T., Kumar, A., Raghava, G.P.S., Katti, S.B., Haq, W., and Sarma, P.U. (2009). Prophylactic and Therapeutic Potential of Asp f1 Epitopes in Naïve and Sensitized BALB/c Mice. **Immune Network** 9, 179.
54. Arora, P.K., Kumar, M., Chauhan, A., Raghava, G.P., and Jain, R.K. (2009). OxDBase: a database of oxygenases involved in biodegradation. **BMC research notes** 2, 67.
55. Vivona, S., Gardy, J.L., Ramachandran, S., Brinkman, F.S., Raghava, G., Flower, D.R., and Filippini, F. (2008). Computer-aided biotechnology: from immuno-informatics to reverse vaccinology. **Trends in biotechnology** 26, 190-200.
56. Raghava, H.J., Hwang DJ (2008). ECGpred: Correlation and prediction of gene expression from nucleotide sequence. **The Open Bioinformatics Journal** 2, 64-67.
57. Kush, A., and Raghava, G. (2008). AC2DGel: analysis and comparison of 2D gels. **Journal of Proteomics & Bioinformatics** 1, 43-46.
58. Kalita, M.K., Nandal, U.K., Pattnaik, A., Sivalingam, A., Ramasamy, G., Kumar, M., Raghava, G.P., and Gupta, D. (2008). CyclinPred: a SVM-based method for predicting cyclin protein sequences. **PLoS one** 3, e2605\_2601-e2605\_2612.
59. Vidyasagar, M., and Balakrishnan, N. (2007). BioSuite: A comprehensive bioinformatics software package (A unique industry-academia collaboration). **Current Science** 92, 29-38.
60. Pashov, A., Monzavi-Karbassi, B., Raghava, G., and Kieber-Emmons, T. (2007). Peptide mimotopes as prototypic templates of broad-spectrum surrogates of carbohydrate antigens for cancer vaccination. **Critical Reviews™ in Immunology** 27.
61. Greenbaum, J.A., Andersen, P.H., Blythe, M., Bui, H.H., Cachau, R.E., Crowe, J., Davies, M., Kolaskar, A., Lund, O., and Morrison, S. (2007). Towards a consensus on datasets and evaluation metrics for developing B-cell epitope prediction tools. **Journal of Molecular Recognition** 20, 75-82.
62. Raghava, G., and Barton, G.J. (2006). Quantification of the variation in percentage identity for protein sequence alignments. **BMC bioinformatics** 7, 415.
63. Kim, J.K., Raghava, G., Bang, S.-Y., and Choi, S. (2006). Prediction of subcellular localization of proteins using pairwise sequence alignment and support vector machine. **Pattern Recognition Letters** 27, 996-1001.
64. Raghava, G. (2006). MANGO: prediction of Genome Ontology (GO) class of a protein from its amino acid and dipeptide composition using nearest neighbor approach. **CASP5**. 26–30.
65. Raghava, G.P., and Han, J.H. (2005). Correlation and prediction of gene expression level from amino acid and dipeptide composition of its protein. **BMC bioinformatics** 6, 59.
66. Genet, H. (2005). The Indian genome variation database (IGVdb): a project overview. **Hum Genet**, 1-11.
67. Sharma, D., Issac, B., Raghava, G., and Ramaswamy, R. (2004). Spectral Repeat Finder (SRF): identification of repetitive sequences using Fourier transformation. **Bioinformatics** 20, 1405-1412.

68. Sarin, J., Raghava, G.P., and Chakraborti, P.K. (2003). Intrinsic contributions of polar amino acid residues toward thermal stability of an ABC-ATPase of mesophilic origin. **Protein Science** 12, 2118-2120.
69. Raghava, G., Searle, S.M., Audley, P.C., Barber, J.D., and Barton, G.J. (2003). OXBench: a benchmark for evaluation of protein multiple sequence alignment accuracy. **BMC bioinformatics** 4, 47.
70. Kaur, H., and Raghava, G. (2003). BTEVAL: A Server for Evaluation of  $\beta$ -Turn Prediction Methods. **Journal of bioinformatics and computational biology** 1, 495-504.
71. Bhasin, M., and Raghava, G. (2003). Prediction of promiscuous and high-affinity mutated MHC binders. **Hybridoma and hybridomics** 22, 229-234.
72. Singh, H., and Raghava, G. (2002). Matrix Optimization Technique for Predicting MHC binding Core. **Biotech Software and Internet Report** 3, 146.
73. Singh, H., and Raghava, G. (2002). Detection of Orientation of MHC Class II Binding Peptides Using Bioinformatics Tools. **Biotech Software & Internet Report** 3, 146-150.
74. Raghava, G. (2002). APSSP2: A combination method for protein secondary structure prediction based on neural network and example based learning. **CASP5**. A-132.
75. Raghava, G., and Agrewala, J.N. (2001). A Web-based Method for Computing Endpoint Titer and Concentration of Antibody/Antigen. **Biotech Software & Internet Report** 2, 196-197.
76. Raghava, G. (2001). PDWSB: Public Domain Web Servers in Biology. **Biotech Software & Internet Report** 2, 152-153.
77. Raghava, G. (2001). PDSB: Public domain software in biology. **Biotech Software & Internet Report** 2, 154-156.
78. Raghava, G. (2001). A web server for computing the size of DNA/protein fragments using a graphical method. **Biotech Software & Internet Report** 2, 198-200.
79. Raghava, G. (2001). A graphical web server for the analysis of protein sequences and alignment. **Biotech Software & Internet Report** 2, 254-257.
80. Raghava, G. (2000). Protein secondary structure prediction using nearest neighbor and neural network approach. **CASP 4, 75-76**.
81. Nihalani, D., Raghava, G., and Sahni, G. (1997). Mapping of the plasminogen binding site of streptokinase with short synthetic peptides. **Protein science** 6, 1284-1292.
82. Ragliava, G., and Agrewala, J.N. (1994). Method for determining the affinity of monoclonal antibody using non-competitive ELISA: a computer program. **J Immunoassay** 15, 115-128.
83. Agrewala JN, Raghava GP, Mishra GC (1993) Measurement and computation of murine interleukin-4 and interferon-gamma by exploiting the unique abilities of these lymphokines to induce the secretion of IgG1 and IgG2a. **J Immunoassay** 14:83-97.
84. Tripathy, S., Balasubramanian, R., Raghava, GP, and Chatterjee, J. (1988). Microprocessor based active and reactive power measurement. **Journal of the Institution of Engineers** 69, 73-77.

## Book Chapters

1. Jain, S., Dhall, A., Patiyal, S., and Raghava, G.P. (2023). In Silico Tool for Identification, Designing, and Searching of IL13-Inducing Peptides in Antigens. **Methods Mol Biol.** 2673:329-338.
2. Dhall, A., Patiyal, S., Sharma, N., Usmani, S.S., and Raghava, G.P. (2023). A Web-Based Method for the Identification of IL6-Based Immunotoxicity in Vaccine Candidates. **Methods Mol Biol.** 2673:317-327
3. Kumar, V., and Raghava, G.P. (2022). In Silico Design of Chemically Modified Cell-Penetrating Peptides. Cell Penetrating Peptides: **Methods Mol Biol.** 2383:63-71.
4. Nagpal, G., Chaudhary, K., Dhanda, S.K., and Raghava, G.P.S. (2017). Computational prediction of the immunomodulatory potential of RNA sequences. RNA Nanostructures: **Methods Mol Biol.** 1632:75-90.
5. Gautam, A., Chaudhary, K., Kumar, R., Gupta, S., Singh, H., and Raghava, G.P. (2016). Managing Drug Resistance in Cancer: Role of Cancer Informatics. **Methods Mol Biol.** 1395:299-312.
6. Singh, H., Gupta, S., Gautam, A., and Raghava, G.P. (2015). Designing B-Cell Epitopes for Immunotherapy and Subunit Vaccines. Peptide Antibodies: **Methods Mol Biol.** 1348:327-40.
7. Gupta, S., Kapoor, P., Chaudhary, K., Gautam, A., Kumar, R., and Raghava, G.P. (2015). Peptide Toxicity Prediction. **Methods Mol Biol.** 1268:143-57.
8. Gautam, A., Chaudhary, K., Kumar, R., and Raghava, G.P.S. (2015). Computer-aided virtual screening and designing of cell-penetrating peptides. **Methods Mol Biol.** 1324:59-69. .
9. Ansari, H.R., and Raghava, G.P. (2013). In Silico Models for B-Cell Epitope Recognition and Signaling. **Methods Mol Biol.** 993:129-38
10. Saha, S., and Raghava, G.P. (2007). Predicting virulence factors of immunological interest. **Methods Mol Biol.** 409:407-15.
11. Saha, S., and Raghava, G.P. (2007). Searching and mapping of B-cell epitopes in Bcipep database. **Methods Mol Biol.** 409:113-24.
12. Saha, S., and Raghava, G.P. (2007). Prediction methods for B-cell epitopes. **Methods Mol Biol.** 409:387-94.
13. Lata, S., Bhasin, M., and Raghava, G.P. (2007). Application of machine learning techniques in predicting MHC binders. **Methods Mol Biol.** 409:201-15.
14. Bhasin, M., Lata, S., and Raghava, G.P. (2007). Searching and mapping of T-cell epitopes, MHC binders, and TAP binders. **Methods Mol Biol.** 409:95-112.
15. Bhasin, M., Lata, S., and Raghava, G. (2007). TAPPred prediction of TAP-binding peptides in antigens. **Methods Mol Biol.** 409:381-6.
16. Bhasin, M., and Raghava, G. (2006). Computational Methods in Genome Research. **Applied Mycology and Biotechnology, (Elsevier)**, pp. 179-207.
17. Issac, B., and Raghava, G.P. (2005). FASTA Servers for Sequence Similarity Search. In **The Proteomics Protocols Handbook, (Humana Press)**, pp. 503-525.
18. Saha, S., and Raghava, G.P.S. (2004). BcePred: prediction of continuous B-cell epitopes in antigenic sequences using physico-chemical properties. **Lecture Notes in Computer Science**, 3239:197-204.

List of major Copyrights

1. Raghava, G.P.S. (1996) ASSP: A computer program for comparision of observed and predicted protein secondary structure. L-15582/96.
2. Raghava, G.P.S. (1996) A computer program for analysing and creating protein secondary structure database. L-15658/96.
3. Raghava, G.P.S and Agrawal, P. A (1997) Software for phylogncitic identification of microorganisms. C R. 1/97, date 11.3.97
4. Raghava, G.P.S (2001) A computer program for assisting the user in using protein modelling software package (PMOD 1.0) . SW-393/2001, date 08/02/2001
5. Kaur, H. and Raghava, G.P.S. (2002) BETATPRED: Software for predicting b -turns using statistical algorithm. SW-1162/2003
6. Raghava, G.P.S. (2002) DNASIZE: A software package for computing DNA/Protein fragments. SW-1156/2003.
7. Issac, B., Singh, H., Kaur, H. and Raghava, G.P.S. (2002) FTG: Software Package for Predicting Gene in DNA using Fast Fourier Transform. SW-1154/2003.
8. Issac, B. and Raghava, G.P.S. (2002) GWBLAST: Software Package for Genome Wide Similarity Search using BLAST. SW-1149/2003
9. Issac, B. and Raghava, G.P.S. (2002) GWFasta: Computer program for genome wide FASTA search. SW-1143/2003.
10. Raghava, G.P.S. (2002) LibNet: Software Package for Managing Library Resources and Accessing via Internet. SW-1155/2003.
11. Singh, H. and Raghava, G.P.S. (2002) MHCBind: Evaluation of MHC Binding Peptide Prediction Algorithms. SW-1160/2003.
12. Singh, H. and Raghava, G.P.S. (2002) MOT: Matrix Optimization Technique for identifying the MHC binding core. SW-1159/2003
13. Raghava, G.P.S. (2002) PCLASS: Computer Program for predicting structural class of protein via Internet. SW-1157/2003
14. Raghava, G.P.S. (2002) PDSB: Software Package for Managing Public Domain Software in Biology. SW-1148/2003.
15. Raghava, G.P.S. (2002) PDWSB: Software Package for creating and managing Biological Web Servers. SW-1152/2003.
16. Singh, H. and Raghava, G.P.S. (2002) ProPred: Software package for predicting promiscuous MHC class-II binding peptides. SW-1163/2003
17. Singh, H. and Raghava, G.P.S. (2002) ProPred-I: Software package for predicting promiscuous MHC Class-I binding peptides. SW-1161/2003
18. Raghava, G.P.S. (2002) PSAweb: Software package for Analyzing of Protein Sequence and Multiple Alignment. SW-1158/2003.
19. Bhasin, M. and Raghava, G. P.S. (2003) MHCBN: A software package for managing data of Immunologically related peptides. SW-1151/200
20. Bhasin, M. and Raghava, G. P.S. (2003) HLA-DR4Pred: An SVM and ANN based software for the prediction of HLA-DRB0401 binding peptides (Submitted).
21. Saha, H. Bhasin, M. and Raghava, G. P.S. (2003) Bcipep: A software package for management of B cell epitopes. SW-1851/200
22. Bhasin, M. and Raghava, G. P.S. (2002) A Webserver for Prediction of Promiscuous And High Affinity Mutated MHC Binders (Submitted).
23. Bhasin, M. and Raghava, G. P.S. (2002) TAPPred: A software package for predicting TAP binding affinity of peptides via internet. SW-1847/2005.
24. Kaur, H. and Raghava, G.P.S. (2003) AlphaPred: A software for prediction of Alpha-turns in proteins (Submitted)
25. Kaur, H. and Raghava, G.P.S. (2003) BetatPred2: A software for prediction of beta-turns in proteins from multiple alignment using neural network (Submitted).
26. Kaur, H. and Raghava, G.P.S. (2003) BetaTurns: A software for prediction of beta-turn types in proteins from evolutionary information using neural network (Submitted).
27. Kaur, H. and Raghava, G.P.S. (2003) Ar\_NHPred: A software for prediction of aromatic-backbone NH interactions in proteins. SW-1850/2005.
28. Issac, B and G.P.S. Raghava (2003) SVMgene: Predicting protein coding regions in human genomic DNA using SVM. SW-1852/2005.
29. Kaur, H. and Raghava, G.P.S. (2003) CHPredict: A software for prediction of C-H...O and C-H...( interactions in proteins using recurrent neural network (Submitted).
30. Bhasin, M. and Raghava, G. P. S. (2005) Pcleavage: A SVM based Method for Prediction of Constitutive and Immuno proteasome Cleavage Sites in Antigenic Sequences. SW-1950/2005.

31. Bhasin, M. and Raghava, G. P. S. (2004) ESLpred: SVM Based Method for Subcellular Localization of Eukaryotic Proteins using Dipeptide Composition and PSI-BLAST. SW-2104/2005.
32. Bhasin, M. and Raghava, G. P. S. (2004) GPCRpred: An SVM Based Method for Prediction of families and subfamilies of G-protein coupled receptors Nucleic. SW-2108/2005.
33. Kush, A. and Raghava, G. P. S. (2008) AC2DGel: Analysis and Comparison of 2D Gels. SW-2123/2005
34. Bhasin, M. and Raghava, G. P. S. (2005) GPCRsclass : A web tool for classification of amine type of G-protein coupled Receptors. SW-1947/2005.
35. Saha, S. and Raghava, G. P. S. (2006) VICMpred: SVM-based method for the prediction of functional proteins of gram-negative bacteria using amino acid patterns and composition. SW-2287/2005.
36. Singh, H. and Raghava, G. P. S. (2007) Prediction and mapping of promiscuous MHC class II binders in an antigen sequence. SW-2286/2005
37. Saha, S. and Raghava, G. P. S. (2006) AlgPred: Prediction of allergenic proteins and mapping of IgE epitopes. SW-3013/2006.
38. Kumar, M., Thakur, V. and Raghava, G. P. S. (2008) COPid: composition based protein identification. SW-3074/2005.
39. Bhasin, M. and Raghava, G. P. S. (2004) Classification of nuclear receptors based on amino acid composition and dipeptide composition. SW-2124/2005.
40. Aarti Garg, Manoj Bhasin, and Gajendra P. S. Raghava (2005). SVM-based method for subcellular localization of human proteins using amino acid compositions, their order and similarity search. SW-2269/2005.
41. Saha, S. and Raghava, G. P. S. (2007) Prediction of neurotoxins based on their function and source. SW-2352/2005.
42. Saha, S. and Raghava, G. P. S. (2007) Prediction of bacterial proteins. SW-2652/2005.
43. Rashid M., Saha S. and Raghava, G. P. S. (2007) TBpred: A SVM based subcellular localization prediction method for Mycobacterial proteins. SW-3635/2007
44. Rakesh Kaundal and Raghava, G. P. S. RSLpred: A svm based method for subcellular localization prediction of rice proteins. SW-3638/2007.
45. Ahmed Firoz, Kumar M. and Raghava G. P. S. PolyApred: SVM based method for predicting of polyadenylation signals in human DNA sequence. SW-3637/2007.
46. Ahmed Firoz, Singh J. and Raghava G. P. S. CDpred: Prediction of cleavage site of Dicer using support vector machine. (Submitted)
47. Lata, S. and Raghava, G. P. S. (2008) PRRDB: A comprehensive database of Pattern-Recognition Receptors and their ligands (Submitted).
48. Ahmed Firoz, Ansari H.R. and Raghava G. P. S. RISCbinder: Prediction of guide strand of microRNAs from its sequence and secondary structure. (Submitted).
49. A suite of programs for computer-aided vaccine design. SW-2264/2005.
50. Ahmed Firoz, Singh J. and Raghava G. P. S. (2009) CDpred: Prediction of cleavage site of Dicer using support vector machine. (SW-4017/2009).
51. Lata, S. and Raghava, G. P. S. (2009) PRRDB: A comprehensive database of Pattern-Recognition Receptors and their ligands (SW-4018/2009).
52. Ahmed, F., Ansari, H.R. And Raghava, G.P.S (2009) Prediction of guide strand of microRNAs from its sequence and secondary structure (RISC binder in Short) (SW-4193/2009).
53. Panwar, B. And Raghava, G.P.S (2010) Prediction and classification of AminoacylNRAsyntheases using signature profile-based descriptors (SW-4633/2010).
54. Ansari, H.R. And Raghava, G.P.S (2010) Identification of NAD interacting residues in proteins (SW-4637/2010).
55. Chauhan, J.S. , Mishra, N.K. And Raghava, G.P.S (2010) GTPbinder: A web based tool for prediction of GTP binding residue in protein sequence (SW-4638/2010).
56. Mishra, N.K and Raghava, G.P.S (2010) FADPred: Prediction of FAD interacting amino acid residue using evolutionary information and SVM (SW-4639/2010)
57. Chauhan, J.S., Mishra, N.K. And Raghava, G.P.S (2010) ATPrint: Prediction of ATP interacting amino acid residue of proteins by SVM and PSSM (SW-4636/2010).
58. Lata, S. , Mishra, N.K and Raghava, G.P.S (2010) AntiBP2: Improved version of antibacterial peptide prediction (SW-4634/2010).

59. Rashid, M and Raghava, G.P.S (2010) MycoPrint: Prediction of protein-protein interaction in *Mycobacterium tuberculosis* (SW-4635/2010).
60. Kumar, S. And Raghava, G.P.S :GenomeABC: A platform for benchmarking of genome assemblers (CR No. 035CR2011).
61. Sharma, A. ,Singla, D. , Rashid M and Raghava, G.P.S (2011) DESTAMP: Designing of stable antibacterial mutant peptides (CR No. 036CR2011).
62. Mishra, N.K, Singla, D. ,Agarwal, S. And Raghava G.P.S (2011)ToxiPred: A server for prediction of aqueous toxicity of small chemical molecules in *T. Pyriformis* (CR No. 017CR2011).
63. Panwar, B. And Raghava, G.P.S (2011) Prediction and Classification of Nucleic Acid Interacting Residues in a Protein using Composition Profile of Patterns (CR No. 018CR2011).
64. Rahman, H and Raghava G.P.S (2011) CBTOPE for the identification of conformational B-cell Epitopes in an antigen from its primary sequence. (CR No. 016CR2010 ).
65. Singh, H. ,Agarwal, S. , Ansari, H.R and Raghava, G.P.S (2011)SfePred: Prediction of the year of evolution of swine flu (CR No. 005CR2010).
66. Ansari, H.R., Agarwal, S. And Raghava, G.P.S (2011) NPTOPE for the prediction of non-peptide epitopes using QSAR based Random Forest model (CR No. 013CR2010).
67. Agarwal, S, Mishra, N.K and Raghava, G.P.S (2011)PreMieR: Prediction of Mannose Interacting Residues (CR No. 011CR2010).
68. Panwar, B. And Raghava, G.P.S (2011) Discrimination between cytosolic and mitochondrialtRNAsynthetases (CR No. 039CR2010).
69. Sharma, A, Singla, D., Rashid, M. and Raghava, G.P.S. (2011) "DESTAMP: Designing of stable antibacterial mutant peptides (Applied).
70. Ansari, H.R.,Singla, D., Raghava, G.P.S. (2011) "TLR4hi- a software for computing antagonist of human TLR4".
71. Panwar,B., Gupta, S., and Raghava, G.P.S. (2012) "VitaPred- Software for the sequence based prediction of vitamin interacting residues using evolutionary information (Applied).
72. Singh, H., Ansari, H.R. and Raghava, G.P.S. (2012) "LBtope: Improved method for linear B-cell epitope prediction using antigen's primary sequence (Applied).
73. Dhanda, S.,K., Singla, D., Mondal, A.,K. and Raghava, G.P.S. (2012) "Drugmint: Knowledge based approach for predicting drug-likeness of a molecule (Applied).
74. Chhauhan, J.,S., Bhat, A.,H., Rao, A. and Raghava, G.P.S. (2012) "GlycoPP: A Webserver for Prediction of N- O-Glycosites in Prokaryotic Protein Sequences (Applied).
75. Singh, H., Singh, S., and Raghava, G.P.S. (2013) "PEP2D: Bayesian based approach for predicting secondary structure of peptides using evolutionary information (Applied).
76. Chaudhary K, Kumar R, Singh S, Tuknait A, Gautam A, Mathur D, Anand P, Varshney G C, and Raghava GPS(2015) HemoPI: A web server and mobile app for computing hemolytic potency of peptides (Applied)

## 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
mhcbs	13	366192	4760496	1586832	793416	4046
rnapred	7	633188	4432316	1477438	738719	3767
cancerdr	4	916792	3667168	1222389	611194	3117
cpps	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
lbtop	3	774590	2323770	774590	387295	1975
propred	14	155590	2178440	726146	363073	1851
pepstr	9	229592	2066328	688776	344388	1756
hmrb	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
ccp	4	332040	1328160	442720	221360	1128
nppred	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
btxpred	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
gwblast	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
prrdb	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
paaint	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>