# **Curriculum Vitae**

# Gajendra P. S. Raghava

## PERSONAL DETAILS:

Name: Gajendra P. S. Raghava Current Position: Professor Date of Birth: 25th May 1963

Organization/Institute: Indraprastha Institute of Information Technology,

Web Site <a href="http://webs.iiitd.edu.in/raghava/">http://webs.iiitd.edu.in/raghava/</a>

Google Scholar: https://scholar.google.co.in/citations?user=XK5GUiYAAAAJ&hl=en

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# **EDUCATION QUALIFICATION & PROFESSIONAL EXPERIENCE**

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

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

## Positions held in chronological order

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

## Significant foreign assignments

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

## MAJOR PROJECTS/FUNDINGS

# (Major grants/project in last 10 years)

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 head this project from 1994 to 2016 and got funding of around Rs 5 crores from DBT over the years.

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. Following site may provide more information about this project GENESIS. This project total budget was around Rs 50 crores.

**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.

Advanced Centre for Protein Informatics, Science, Engineering & Technology: This is a facility creation project of CSIR, coordinated by CSIR-IMTECH (Nodal Officer: G P S Raghava) under 11th five-year plan (2007-11). The proposal is 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.

# **RESEARCH CONTRIBUTION**

#### Significant contributions to science and/or technology

Raghava contributed significantly in the field of bioinformatics and chemoinformatics particularly in t computer-aided drug and vaccine design. In contrast to traditional researchers where a scientist contributed particular problem or field; He contributed to multiple problems/fields important for translational me group developed more than 200 web servers, databases and software packages, which is highest contributions in the world. Following are major contributions.

• Potential Drug Targets: His group developed software for annotating genomes at nucleotic

as at protein level, in order to identify potential drug targets. Highly accurate and novel methods to been developed for predicting genes and Spectral Repeats in genomes. These methods to published in the top journals in the field of bioinformatics (e.g. *Genome Research; Bioinform* genomics. Raghava's group developed number of novel methods for classifying and receptors (G-protein coupled receptor (GPCR), nuclear receptors), toxins and virulent prot group developed method for predicting secondary structure (regular as well as irregular secondary structure (e.g. beta-hairpins, beta-barrels) and tertiary structure (ab initio me bioactive peptides). The performance of their best secondary structure prediction method w within the top methods in the world, according to the community wide competitions lil CAFASP and EVA. Raghava's group is developing computation resources for drug discovery an in-silico modules of Open Source Drug Discovery(OSDD) where his group is collecting, and developing computational resources for designing therapeutic molecules. His group is refor promoting open source in the field of chemoinformatics and pharmacoinformatics. In a development of software for designing small molecules, group also developed for designentrating, tumor homing, antibacterial peptides etc.

- Computer-Aided Vaccine Design: Since 2001, his group is developing methods for various component required for understand immune system and for designing subunit vac primary/reference immunological databases (MHCBN, BCIpep, PRRDB, AntigenDB, H PolysacDB) have been developed by his group. In order to predict CTL epitopes with high algorithams were developed for each component of its pathway, it includes i) Propred1 for j of binders for 47 MHC class I alleles; ii) TAPpred for predict TAP binding peptides; iii) Pck predicting protease clevage sites. First time group developed method to predict conformatio epitopes in antigen sequence. Overall more than 20 databases and web servers have been developed immunoinformatics.
- Experimental Validation of Predictions: His group is known for developing in silico tools heavily used by scientific community. Recently group also integrated theortical and exprescience to solve real life problems. His group discovered novel cell penetrating peptides integrative approach, which have better efficacy than existing peptides. These peptides capability to deliver proteins and peptides inside human cells and skin layer. These peptides patented and published. In addition his group sequenced whole genome of number of and annotated important pathways with experimental validation.

#### Research in term of Impact factor

Raghava's group has developed more than 250 in silico products (web servers and databases), each product is based on novel algorithm or data. Most of publications based on these in silico products are highly cited. Students and scientific community in the field of education, vaccine and drug discovery heavily use these services. Following is summary of these publications that includes name of journal, journals impact factor, number of papers published by group and total impact (impact x papers)

Name of Journal	Impact Factor*	No. of Papers	Total Impact	Comment
Science	34.6	1	34.7	
Genome Research	14.6	1	14.6	*Impact factor is either latest if
Trends in Biotech.	11.9	1	11.9	paper published long time back or
Briefings in Bioinformatics	9.6	1	9.6	maximum impact factor if multiple
Nucleic Acids Res.	9.1	16	145.6	papers published in different years.
Journal Biol. Chemistry	6.4	3	19.2	
Bioinformatics	6.0	11	66.0	It excludes impact factor of papers
BMC Bioinformatics	5.4	23	124.2	published in new journals or
Scientific Reports (Nature)	5.6	22	123.2	protocols
Biology Direct	4.7	7	32.9	
BMC Genomics	4.4	5	22.0	
Plos One	4.4	21	92.4	
Proteins	4.4	7	30.8	
Protein Science	4.1	5	20.5	
Front. Microbiol.	4.1	2	8.2	
Other journals	~3.0	80	240	
Total Impact factor (around) of pa	pers		~1000	

#### Citation information

Total citations on all papers	~15200
Maximum citation of a single paper	840
Papers with more than 200 citations	16
Papers with more than 100 citations	45
Papers with more than 10 citations (g-index)	191
Average Citation per paper	~40
h-index	67

# **TEACHING AND HUMAN RESOURCE DEVELOPMENT (HRD)**

Raghava works at two organization (CSIR-IMTECH and IIIT Delhi) during the current position of professor. Following is brief description of contribution at two organizations.

#### **CSIR-IMTECH**

- Long term training: More than 80 students have been trained (PA, RA, Summer trainees) that includes 36 Ph.D students (24 completed).
- **Short Training:** More than 700 students got short term training as workshop/conference participants. Two international & more than 10 national workshop/training/conference were organized.
- **Bioinformatics Course**: Taught around 200 pre-phd students over the years; full one session. In addition, we are organizing small training programs for faculty and student of IMTECH from last 20 years.
- **Virtual skill development**: In addition to direct training, we are providing training to users via our online computational resources. All tutorials/ documents/presentations related to bioinformatics are available from our sites. Under GPSR package we provide PERL code required to write core script in the field of computational biology. All over the world students and young faculties are using theses source codes for learning as well as for developing their own software packages.

• Specialized Trainings: A customized training was organized for employees of a private company from South Korea in the year of 2002, for which we received Rs 4.55 lakhs. We also organized training for Department of Electronics (DOE) in year 2003, on PERL in Bioinformatics for which we received Rs 2.80 lakhs.

#### **IIIT Delhi**

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 very popular among students particularly in B.Tech/M.Tech computer science students, in last semester more than 100 students join the course. Based on feedback of students, I am getting "Teaching Excellence Award" every year at IIIT Delhi. In addition, I got "Outstanding Educator Award" based on nomination by graduating BTech and MTech batches. A number of workshop/conferences organized to trained students outside IIIT Delhi. Number of M.Tech/B.Tech students completed their thesis, IP, IS and Capstone project in last two years.

## **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 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. The main purpose of this web portal is to provide help to biologist working in the field of vaccine development, drug designing, etc. The servers help biologist's in identifying potential vaccine candidates and hence save time and money. Overall aim of the web portal is to provide scientific computation and resources required in the healthcare sector. Indian researchers had contributed significantly in the field of informatics, particularly in the field of biomedicine. In order to provide visibility to web servers/software developed by Indian scientific community, we provide a link to these resources. This web portal is heavily used by the scientific community, getting thousands of hits per day.

• 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 at IMTECH, Chandigarh. We successfully install and set more than 200 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 ( <a href="http://webs.iiitd.edu.in/raghava/">http://webs.iiitd.edu.in/raghava/</a>).

## **HONORS & AWARDS**

#### > Fellow of National Academies

- Fellow of National Academy of Sciences, India
- Fellow of Indian Academy of Sciences, Banglore

## > Major National Awards

- 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. Lakshmipat Singhania-IIM Lucknow National Leadership Awards 2011 (Young Leader in category of Science and Technology)
- 6. One paper listed in top 70 highly cited papers (ranked 18) published by CSIR scientists in last 70 years
- 7. Sun Pharma Research Award 2018 by Sun Pharma Science Foundation
- 8. Scientist Award 2019 by Organisation of Pharmaceutical Producers of India

#### **➤** Major International recognition/awards

- Listed in "The World's Most Influential Scientific Minds" by Thompson Reuters. This list contain 3200 individuals who published the greatest number of highly cited papers in one of 21 broad fields, 2002-2012. Highly cited papers rank in top 1% by citations for their field and year of publication. Seven Indian scientist have been listed in above list. <a href="http://sciencewatch.com/sites/sw/files/sw-article/media/worlds-most-influential-scientific-minds-2014.pdf">http://sciencewatch.com/sites/sw/files/sw-article/media/worlds-most-influential-scientific-minds-2014.pdf</a>
- 2. Thomson Reuters Research Excellence India Research Front Awards 2009

## Annexure I

# **List of Patents**

- 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

# **Research Publications of Raghava**

- 1. Bhalla, S., Kaur, H., Kaur, R., Sharma, S., & Raghava, G. P. S. (2020). Expression based biomarkers and models to classify early and late-stage samples of Papillary Thyroid Carcinoma. *PloS One*, *15*(4), e0231629. https://doi.org/10.1371/journal.pone.0231629
- 2. Dhall, A., Patiyal, S., Kaur, H., Bhalla, S., Arora, C., & Raghava, G. P. S. (2020). Computing Skin Cutaneous Melanoma Outcome from the HLA-alleles and Clinical Characteristics. *Frontiers in Genetics*, 11.
- 3. Kaur, D., Arora, C., & Raghava, G. P. S. (2020). A hybrid model for predicting pattern recognition receptors using evolutionary information. *Frontiers in Immunology*, 11, 71.
- 4. Kaur, H., Bhalla, S., Kaur, D., & Raghava, G. P. S. (2020). CancerLivER: a database of liver cancer gene expression resources and biomarkers. *Database*, 2020.
- 5. Kumar, R., Lathwal, A., Kumar, V., Patiyal, S., Raghav, P. K., & Raghava, G. P. S. (2020). CancerEnD: A database of cancer associated enhancers. *Genomics*. https://doi.org/10.1016/j.ygeno.2020.04.028
- 6. Kumar, V., Kumar, R., Agrawal, P., Patiyal, S., & Raghava, G. P. S. (2020). A Method for Predicting Hemolytic Potency of Chemically Modified Peptides From Its Structure. *Frontiers in Pharmacology*, 11, 54.
- 7. Lathwal, A., Kumar, R., & Raghava, G. P. S. (2020). Computer-aided designing of oncolytic viruses for overcoming translational challenges of cancer immunotherapy. *Drug Discovery Today*. https://doi.org/10.1016/j.drudis.2020.04.008
- 8. Mason, M. J., Schinke, C., Eng, C. L. P., Towfic, F., Gruber, F., Dervan, A., White, B. S., Pratapa, A., Guan, Y., Chen, H., & others. (2020). Multiple Myeloma DREAM Challenge reveals epigenetic regulator PHF19 as marker of aggressive disease. *Leukemia*, 1–9.
- 9. Patiyal, S., Agrawal, P., Kumar, V., Dhall, A., Kumar, R., Mishra, G., & Raghava, G. P. S. (2020). NAGbinder: An approach for identifying N-acetylglucosamine interacting residues of a protein from its primary sequence. *Protein Science*, 29(1), 201–210.
- 10. Agrawal, P., Kumar, S., Singh, A., Raghava, G. P. S., & Singh, I. K. (2019). NeuroPIpred: a tool to predict, design and scan insect neuropeptides. *Scientific Reports*, 9(1), 1–12.
- 11. Agrawal, P., Mishra, G., & Raghava, G. P. S. (2019). 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. https://doi.org/10.3389/fphar.2019.01690
- 12. Agrawal, P., Patiyal, S., Kumar, R., Kumar, V., Singh, H., Raghav, P. K., & Raghava, G. P. S. (2019). ccPDB 2.0: an updated version of datasets created and compiled from Protein Data Bank. *Database*, 2019.
- 13. Agrawal, P., Singh, H., Srivastava, H. K., Singh, S., Kishore, G., & Raghava, G. P. S. (2019). Benchmarking of different molecular docking methods for protein-peptide docking. *BMC Bioinformatics*, 19(13), 426.
- 14. Akhter, S., Kaur, H., Agrawal, P., & Raghava, G. P. S. (2019). RareLSD: a manually curated database of lysosomal enzymes associated with rare diseases. *Database*, 2019.
- 15. Bhalla, S., Kaur, H., Dhall, A., & Raghava, G. P. S. (2019). Prediction and analysis of skin cancer progression using genomics profiles of patients. *Scientific Reports*, 9(1), 1–16.
- 16. Brown, P., Tan, A.-C., El-Esawi, M. A., Liehr, T., Blanck, O., Gladue, D. P., Almeida, G. M. F., Cernava, T., Sorzano, C. O., Yeung, A. W. K., & others. (2019). Large expert-curated database for benchmarking document similarity detection in biomedical literature search. *Database*, 2019.
- 17. Kaur, D., Patiyal, S., Sharma, N., Usmani, S. S., & Raghava, G. P. S. (2019). PRRDB 2.0: a comprehensive database of pattern-recognition receptors and their ligands. *Database*, 2019.

- 18. Kaur, H., Bhalla, S., & Raghava, G. P. S. (2019). Classification of early and late stage liver hepatocellular carcinoma patients from their genomics and epigenomics profiles. *PloS One*, 14(9).
- 19. Kumar, R., Nagpal, G., Kumar, V., Usmani, S. S., Agrawal, P., & Raghava, G. P. S. (2019). HumCFS: A database of fragile sites in human chromosomes. *BMC Genomics*, *19*(9), 985.
- 20. Kumar, R., Patiyal, S., Kumar, V., Nagpal, G., & Raghava, G. P. S. (2019). In Silico Analysis of Gene Expression Change Associated with Copy Number of Enhancers in Pancreatic Adenocarcinoma. *International Journal of Molecular Sciences*, 20(14), 3582.
- 21. Lathwal, A., Arora, C., & Raghava, G. P. S. (2019). Prediction of risk scores for colorectal cancer patients from the concentration of proteins involved in mitochondrial apoptotic pathway. *PloS One*, *14*(9).
- 22. Raghav, P. K., Kumar, R., Kumar, V., & Raghava, G. P. S. (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(11), e910.
- 23. Usmani, S. S., Agrawal, P., Sehgal, M., Patel, P. K., & Raghava, G. P. S. (2019). ImmunoSPdb: an archive of immunosuppressive peptides. *Database*, 2019.
- 24. Agrawal, P., Raghav, P. K., Bhalla, S., Sharma, N., & Raghava, G. P. S. (2018). Overview of free software developed for designing drugs based on protein-small molecules interaction. *Current Topics in Medicinal Chemistry*.
- 25. Agrawal, P., Bhalla, S., Chaudhary, K., Kumar, R., Sharma, M., & Raghava, G. P. S. (2018). In silico approach for prediction of antifungal peptides. *Frontiers in Microbiology*, *9*, 323.
- 26. Agrawal, P., & Raghava, G. P. S. (2018). Prediction of Antimicrobial Potential of a Chemically Modified Peptide from its Tertiary Structure. *Frontiers in Microbiology*, 9, 2551.
- 27. Kumar, R., Kaur, R., Bhondekar, A. P., & Raghava, G. P. S. (2018). Human Opinion Inspired Feature Selection Strategy for Predicting the Pleasantness of a Molecule. In *Advanced Computational and Communication Paradigms* (pp. 197–205). Springer.
- 28. Kumar, V., Agrawal, P., Kumar, R., Bhalla, S., Usmani, S. S., Varshney, G. C., & Raghava, G. P. S. (2018). Prediction of cell-penetrating potential of modified peptides containing natural and chemically modified residues. *Frontiers in Microbiology*, *9*, 725.
- 29. Mathur, D., Mehta, A., Firmal, P., Bedi, G., Sood, C., Gautam, A., & Raghava, G. P. S. (2018). TopicalPdb: A database of topically delivered peptides. *PloS One*, *13*(2).
- 30. Mathur, D., Singh, S., Mehta, A., Agrawal, P., & Raghava, G. P. S. (2018). In silico approaches for predicting the half-life of natural and modified peptides in blood. *PloS One*, 13(6).
- 31. Nagpal, G., Chaudhary, K., Agrawal, P., & Raghava, G. P. S. (2018). Computer-aided prediction of antigen presenting cell modulators for designing peptide-based vaccine adjuvants. *Journal of Translational Medicine*, 16(1), 181.
- 32. Nagpal, G., Usmani, S. S., & Raghava, G. P. S. (2018). A web resource for designing subunit vaccine against major pathogenic species of bacteria. *Frontiers in Immunology*, 9, 2280.
- 33. Usmani, S. S., Bhalla, S., & Raghava, G. P. S. (2018). Prediction of antitubercular peptides from sequence information using ensemble classifier and hybrid features. *Frontiers in Pharmacology*, 9(AUG). https://doi.org/10.3389/fphar.2018.00954
- 34. Usmani, S. S., Kumar, R., Bhalla, S., Kumar, V., & Raghava, G. P. S. (2018). In Silico Tools and Databases for Designing Peptide-Based Vaccine and Drugs. *Advances in Protein Chemistry and Structural Biology*.
- 35. Usmani, S. S., Kumar, R., Kumar, V., Singh, S., & Raghava, G. P. S. (2018). AntiTbPdb: a knowledgebase of anti-tubercular peptides. *Database*, 2018.

- 36. Baindara, P., Gautam, A., Raghava, G. P. S., & Korpole, S. (2017). Anticancer properties of a defensin like class IId bacteriocin Laterosporulin10. *Scientific Reports*, 7, 46541.
- 37. Bhalla, S., Chaudhary, K., Kumar, R., Sehgal, M., Kaur, H., Sharma, S., & Raghava, G. P. S. (2017). Gene expression-based biomarkers for discriminating early and late stage of clear cell renal cancer. *Scientific Reports*, 7, 44997.
- 38. Bhalla, S., Sharma, S., & Raghava, G. P. S. (2017). Challenges in Prediction of different Cancer Stages using Gene Expression Profile of Cancer Patients. *Proceedings of the 8th ACM International Conference on Bioinformatics, Computational Biology, and Health Informatics*, 602.
- 39. Bhalla, S., Verma, R., Kaur, H., Kumar, R., Usmani, S. S., Sharma, S., & Raghava, G. P. S. (2017). CancerPDF: A repository of cancer-associated peptidome found in human biofluids. *Scientific Reports*, 7(1), 1511.
- 40. Dhanda, S. K., Usmani, S. S., Agrawal, P., Nagpal, G., Gautam, A., & Raghava, G. P. S. (2017). Novel in silico tools for designing peptide-based subunit vaccines and immunotherapeutics. *Briefings in Bioinformatics*, 18(3), 467–478.
- 41. Keller, A., Gerkin, R. C., Guan, Y., Dhurandhar, A., Turu, G., Szalai, B., Mainland, J. D., Ihara, Y., Yu, C. W., Wolfinger, R., & others. (2017). Predicting human olfactory perception from chemical features of odor molecules. *Science*, eaal2014.
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- 43. Nagpal, G., Usmani, S. S., Dhanda, S. K., Kaur, H., Singh, S., Sharma, M., & Raghava, G. P. S. (2017). Computer-aided designing of immunosuppressive peptides based on IL-10 inducing potential. *Scientific Reports*, 7, 42851.
- 44. Pahil, S., Taneja, N., Ansari, H. R., & Raghava, G. P. S. (2017). In silico analysis to identify vaccine candidates common to multiple serotypes of Shigella and evaluation of their immunogenicity. *PloS One*, *12*(8).
- 45. Usmani, S. S., Bedi, G., Samuel, J. S., Singh, S., Kalra, S., Kumar, P., Ahuja, A. A., Sharma, M., Gautam, A., & Raghava, G. P. S. (2017). THPdb: database of FDA-approved peptide and protein therapeutics. *PloS One*, *12*(7).
- 46. Agrawal, P., Bhalla, S., Usmani, S. S., Singh, S., Chaudhary, K., Raghava, G. P. S., & Gautam, A. (2016). CPPsite 2.0: a repository of experimentally validated cell-penetrating peptides. *Nucleic Acids Research*, 44(D1), D1098--D1103.
- 47. Chaudhary, K., Kumar, R., Singh, S., Tuknait, A., Gautam, A., Mathur, D., Anand, P., Varshney, G. C., & Raghava, G. P. S. (2016). A Web Server and Mobile App for Computing Hemolytic Potency of Peptides. *Scientific Reports*, *6*, 22843.
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- 49. Dhanda, S. K., Chaudhary, K., Gupta, S., Brahmachari, S. K., & Raghava, G. P. S. (2016). A web-based resource for designing therapeutics against Ebola Virus. *Scientific Reports*, 6, 24782.
- 50. Dhanda, S. K., Vir, P., Singla, D., Gupta, S., Kumar, S., & Raghava, G. P. S. (2016). A webbased platform for designing vaccines against existing and emerging strains of Mycobacterium tuberculosis. *PloS One*, *11*(4).
- 51. Gautam, A., Chaudhary, K., Kumar, R., Gupta, S., Singh, H., & Raghava, G. P. S. (2016). Managing Drug Resistance in Cancer: Role of Cancer Informatics. *Cancer Drug Resistance: Overviews and Methods*, 299–312.

- 52. Gautam, A., Nanda, J. S., Samuel, J. S., Kumari, M., Priyanka, P., Bedi, G., Nath, S. K., Mittal, G., Khatri, N., & Raghava, G. P. S. (2016). Topical Delivery of Protein and Peptide Using Novel Cell Penetrating Peptide IMT-P8. *Scientific Reports*, 6, 26278.
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# Social Impact of Web Services Developed by Raghava's Group

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

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

# Total social impact in term money is around Rs. 792 crore in year 2015 (Detail is given in table below)

Web-Servers	Online (Years)	Hits/year	Total hits	Pages/visited	Jobs executed	Social Impact (Rs in lakhs)
dnabinder	9	1218502	10966518	3655506	1827753	9321
pcmdb	3	2387778	7163334	2387778	1193889	6088
metapred	6	929140	5574840	1858280	929140	4738
mhcbn	13	366192	4760496	1586832	793416	4046
rnapred	7	633188	4432316	1477438	738719	3767
cancerdr	4	916792	3667168	1222389	611194	3117
cppsite	4	762016	3048064	1016021	508010	2590
bcepred	13	214590	2789670	929890	464945	2371
sarpred	11	232384	2556224	852074	426037	2172
proprint	8	292022	2336176	778725	389362	1985
lbtope	3	774590	2323770	774590	387295	1975
propred	14	155590	2178440	726146	363073	1851
pepstr	9	229592	2066328	688776	344388	1756
hmrbase	8	247044	1976352	658784	329392	1679
npact	3	499456	1498368	499456	249728	1273
glycoep	3	484306	1452918	484306	242153	1234
abcpred	10	139888	1398880	466293	233146	1189
ccpdb	4	332040	1328160	442720	221360	1128
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

Total	880	16993588	93216050	31071990	15535982	79233
antiangiopred	1	8356	8356	2785	1392	7
paaint	2	4988	9976	3325	1662	8
xiapin	1	13030	13030	4343	2171	11
fadpred	6	2682	16092	5364	2682	13
vaccineda	1	17388	17388	5796	2898	14
chemopred	7	2888	20216	6738	3369	17
hivcopred	3	7694	23082	7694	3847	19
dprot	8	3286	26288	8762	4381	22
marspred	4	6682	26728	8909	4454	22

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