

Raj Kumar, Ph.D.

Assistant Professor (Grade-II),
Department of Biotechnology and Bioinformatics, Jaypee
University of Information Technology, Wanknaghat, Solan,
Himachal Pradesh, 173 234, India.

Email: raj.kumar@juit.ac.in, rajkumar250287@gmail.com

Mobile: +91-78762 54267

Academic Profile

Mar 2014- **Ph.D. in Science**, Gyeongsang National University, South Korea.

Aug 2018 Grade: A+

Thesis Title: “Computational Investigations for the Discovery of Selective Inhibitors Targeting Prolyl Oligopeptidase for Neurological Disorders”. (Guide: Prof. Keun Woo Lee)

Aug 2008- **M.Sc. Biotechnology**, Bangalore University, India.

June 2010 Grade: First class

Apr 2005- **B.Sc. (Honours) Biotechnology**, Himachal Pradesh University, India.

Mar 2008 Grade: First class

Research Expertise and Interests

- Computer Aided Drug Design
- Molecular modeling
- Structural Bioinformatics
- Cheminformatics
- Biomolecular Simulations
- Machine Learning for drug discovery

Professional/Research Experience

May 2022- **Assistant Professor (Grade-II)**, Department of Biotechnology and
present Bioinformatics, Jaypee University of Information Technology, Wanknaghat,
India.

Sep 2019- **Assistant Professor (Grade-I)**, Department of Biotechnology and
May-2022 Bioinformatics, Jaypee University of Information Technology, Wanknaghat,
India.

Sep 2018- **Post-Doctoral Fellow**, Institute of Chemical processes (ICP), Seoul National
Sep 2019 University (SNU), South Korea.

Mar 2014- **Graduate Researcher**, Computational Biology and Bioinformatics Lab

Awards and Scholarships

1. ‘**Young Scientist Award**’ by Korean Society for Bioinformatics (KSBI) at the international conference “BIOINFO 2018”, Seoul, Korea, Oct. 31 - Nov. 2, 2018.
2. ‘**Young Pioneer Researcher**’ award, Gyeongsang National University, May 17, 2018.
3. ‘**Best poster presentation**’ award at BIOINFO 2017 GIW/BIOINFO Annual Conference, Samjung Hotel, Seoul, Korea, Oct. 31 - Nov. 3, 2017.
4. ‘**Outstanding Presentation Award**’ for research at the ‘10th Project Presentation Contest in English for Graduate Students and Young Scientists’ hosted by Gyeongsang National University on Dec 12, 2016.
5. ‘**Young Pioneer Researcher**’ award, Gyeongsang National University, May 20, 2015.
6. ‘**Outstanding Presentation Award**’ for research at the ‘9th Project Presentation Contest in English for Graduate Students and Young Scientists’ hosted by Gyeongsang National University on April 23, 2015.
7. Awarded **travel grant** to attend international conference on Computational Advances in Drug Discovery (SBDD2017), Switzerland.
8. Awarded **BK21 plus scholarship** for doctoral research during 2015-2017 by Govt. of Republic of Korea (South Korea).
9. Secured **scholarship** for Biotech Industrial Training Program (**BITP**) during 2010-11.

Publications

- 1 Kumar V, **Kumar R**, Parate S, Danishuddin, Lee G, Kwon M, Jeong S-H, Ro H-S, Lee KW, Kim S-W. Identification of Activated Cdc42-Associated Kinase Inhibitors as Potential Anticancer Agents Using Pharmacoinformatic Approaches. **Biomolecules**. 13(2):217, 2023.
- 2 Sharma T, Sharma A, Xia CL, Lam SS, Khan AA, Tripathi S, **Kumar R**, Gupta VK, Nadda AK. Enzyme mediated transformation of CO₂ into calcium carbonate using purified microbial carbonic anhydrase. **Environmental Research**. 212:113538, 2022.
- 3 Thakur G, Bok EY, Kim SB, Jo CH, Oh SJ, Baek JC, Park JE, Kang YH, Lee SL, **Kumar R**, Rho GJ. Scaffold-free 3D culturing enhance pluripotency, immunomodulatory factors, and differentiation potential of Wharton's jelly-mesenchymal stem cells. **European Journal of Cell Biology**. 101(3):151245, 2022.

- 4 Kumar D, **Kumar R**, Ramajayam R, Lee KW, Shin DS. Synthesis, antioxidant and molecular docking studies of (-)-Catechin derivatives. **Journal of the Korean Chemical Society**. 65(2):106–12, 2021.
- 5 Kumar V, **Kumar R**, Parate S, Yoon S, Lee G, Kim D, et al. Identification of ACK1 inhibitors as anticancer agents by using computer-aided drug designing. **Journal of molecular structure**.1235:130200, 2021.
- 6 Thakur G, **Kumar R**, Kim SB, Lee SY, Lee SL, Rho GJ. Therapeutic status and available strategies in pancreatic ductal adenocarcinoma. **Biomedicines**. 9(2):178, 2021.
- 7 **Kumar R**, Kumar V, Lee KW. A computational drug repurposing approach in identifying the cephalosporin antibiotic and anti-hepatitis C drug derivatives for COVID-19 treatment. **Computers in Biology and Medicine** 130:104186, 2021.
- 8 Barage S, Karthic A, Bavi R, Desai N, **Kumar R**, Kumar V & Lee KW. Identification and characterization of novel RdRp and Nsp15 inhibitors for SARS-COV2 using computational approach. **Journal of Biomolecular Structure and Dynamics**, DOI: 10.1080/07391102.2020.1841026, 2020.
- 9 **Kumar R**, Lee YK, Jho YS. Martini Coarse-Grained Model of Hyaluronic Acid for the Structural Change of Its Gel in the Presence of Monovalent and Divalent Salts. **International Journal of Molecular Sciences**. 21(13):4602, 2020.
- 10 Agrawal K, Shankar J, **Kumar R**, Verma P. Insight into multicopper oxidase laccase from *Myrothecium verrucaria* ITCC-8447: a case study using *in silico* and experimental analysis. **Journal of Environmental Science and Health - Part B Pesticides, Food Contaminants, and Agricultural Wastes**, doi:10.1080/03601234, 2020.
- 11 Zeb A, Kim D, Alam SI, Son M, **Kumar R**, et al. Computational Simulations Identify Pyrrolidine-2,3-dione Derivatives as Novel Inhibitors of Cdk5/p25 Complex to Attenuate Alzheimer's Pathology. **Journal of Clinical Medicine**, 8(5), 746, 2019.
- 12 **Kumar R**, Parameswaran S, Bavi R, Baek A, Minky Son, et al. Investigation of novel chemical scaffolds targeting prolyl oligopeptidase for neurological therapeutics." **Journal of Molecular Graphics and Modelling** 88:92-103, 2019.
- 13 Rampogu S, Park C, Ravinder D, Son M, Baek A, Bavi S, **Kumar R** et al. Pharmacotherapeutics and Molecular Mechanism of Phytochemicals in Alleviating Hormone-Responsive Breast Cancer. **Oxidative Medicine and Cellular Longevity**, Doi.org/10.1155/2019/5189490, 2019.
- 14 Rampogu S, Baek A, Bavi S, Son M, Cao GP, **Kumar R** et al. Identification of Novel Scaffolds with Dual Role as Antiepileptic and Anti-Breast Cancer. **IEEE/ACM Transactions on Computational Biology and Bioinformatics**, Doi: 10.1109/TCBB.2018.2855138, 2018.
- 15 **Kumar R**, Bavi R, Jo MG, Arulalapperumal V, Baek A, et al. New compounds identified through *in silico* approaches reduce the alpha-synuclein expression by inhibiting prolyl oligopeptidase *in vitro*. **Scientific Reports** 7:10827, 2017.

- 16 Rampogu S, Baek A, Son M, Zeb A, Park C, **Kumar R**, *et al.* Computational Exploration for Lead Compounds That Can Reverse the Nuclear Morphology in Progeria. **BioMed Research International** 2017:5270940, 2017.
- 17 Rampogu S, Baek A, Gajula RG, Zeb A, Bavi RS, **Kumar R**, *et al.* Ginger (*Zingiber officinale*) phytochemicals-gingerenone-A and shogaol inhibit SaHPPK: molecular docking, molecular dynamics simulations and in vitro approaches. **Annals of Clinical Microbiology and Antimicrobials** 17:16, 2018.
- 18 Bavi R, **Kumar R***, Rampogu S, Kim Y, Kwon YJ, *et al.* Novel virtual lead identification in the discovery of hematopoietic cell kinase (HCK) inhibitors: application of 3D QSAR and molecular dynamics simulation. **Journal of Receptor and Signal Transduction Research** 37:224-38, 2017.
- 19 Bavi R, **Kumar R***, Choi L, Woo Lee K. Exploration of novel inhibitors for Bruton's tyrosine kinase by 3D QSAR modeling and molecular dynamics simulation. **PLoS One** 11:e0147190, 2016.
- 20 Cao GP, Thangapandian S, Son M, **Kumar R**, Choi YJ, *et al.* QSAR modeling to design selective histone deacetylase 8 (HDAC8) inhibitors. **Archives of Pharmacal Research** 39:1356-69, 2016.
- 21 Bavi R, **Kumar R**, Rampogu S, Son M, Park C, *et al.* Molecular interactions of UvrB protein and DNA from *Helicobacter pylori*: Insight into a molecular modeling approach. **Computers in Biology and Medicine** 75:181-9, 2016.
- 22 **Kumar R**, Son M, Bavi R, Lee Y, Park C, *et al.* Novel chemical scaffolds of the tumor marker AKR1B10 inhibitors discovered by 3D QSAR pharmacophore modeling. **Acta Pharmacologica Sinica** 36:998-1012, 2015.
- 23 Khera P, Singh AK, Priyadarshi R, Khandekar D, Allu RK, Hiremath C, **Kumar R** *et al.* Genetic variability in trait-specific rice germplasm groups based on coefficient of parentage, SSR markers and fertility restoration. **Plant Genetic Resources: Characterization and Utilization** 1–12,2014.
- 24 Sharma VP, Kumar S, Kamal S, **Kumar R** *et al.* Integrated approaches for the management of mycogone perniciosa causing wet bubble disease. **Proceedings of the 8th International Conference on Mushroom Biology and Mushroom Products (ICMBMP8)**536-543, 2014.
- 25 Sharma VP, Kumar S, **Kumar R**, *et al.* Cultural requirements, enzyme activity profile, molecular identity and yield potential of some potential strains of shiitake (*Lentinula edodes*). **Mushroom Research** 22 (2): 105-110, 2013.
- 26 Sharma VP, **Kumar R**, *et al.* Optimizations of some parameters for quality spawn production. **Mushroom Research** 22 (1): 31-36, 2013.

Conference Proceedings

1. Sharma A, **Kumar R**, Jaiswal V. Classification of Heart Disease from MRI Images Using Convolutional Neural Network. **6th IEEE International Conference on Signal Processing, Computing and Control (ISPCC 2k21)**, JUIT, Solan, India, Oct 07-09, 2021.

Book Chapters

1. Sharma A and **Kumar R**. Computational strategies and tools to protein structure prediction, In **Basic Biotechniques for Bioprocess and Bioentrepreneurship**. Elsevier, pp. 225-242, [ISBN: 978-0-12-816109-8] 2023.
2. Sharma A and **Kumar R**. Recent Advancement and Challenges in Deep Learning, Big Data in Bioinformatics. In *Blockchain and Deep Learning: Future Trends and Enabling Technologies* pp. 251-284 Switzerland: Springer Cham. [ISBN : 978-3-030-95419-2], 2022.
2. Singh S, Singh R, Thakur P and **Kumar R**. Phytochemicals, Functionality and Breeding for Enrichment of Cole Vegetables (*Brassica oleracea* L.). **Phytochemicals in Vegetables: A Valuable Source of Bioactive Compounds** pp. 256-295, 2018

Poster presentations (Selected)

1. **Kumar R**. Mutational analysis of microbial carbonic anhydrase for enhanced catalysis. Technologies for Environmental Sustainability and Smart Agriculture, organized by centre of excellence in sustainable technologies for rural development (CESTRD) at Jaypee University of Information Technology, Wagnaghat, Himachal Pradesh, India from September 18 - 19, **2020**.
2. **Kumar R**, Jho Y, Lee KW. Computational investigations for selective prolyl oligopeptidase inhibition for neurological disorders. International Conference on Recent Trends in Biotechnology and Bioinformatics ICBAB-2019 held at Jaypee University of Information Technology, Wagnaghat, Himachal Pradesh, India from August 01 - 03, **2019**.
3. **Kumar R**, Bavi R, Lee KW. Comparative modeling of human tryptophan 2, 3- dioxygenase (TDO) tetramer and optimization of the active site for structure-based drug design. Computational Advances in Drug Discovery (**SBDD2017**), SwissTech Convention Centre, Lausanne, Switzerland, September 05-08, **2017**.
4. **Kumar R**, Bavi R, Baek A, Rampogu S, Lee KW. Comparative modeling of tetrameric form of human tryptophan 2,3-dioxygenase (TDO) and optimization of the active site for structure-based drug design. **Bioinfo 2016**, Incheon Global Campus, Incheon, Korea, August 17-19, **2016**.
5. **Kumar R**, Bavi R, Arulalapperumal V, Lee KW. Novel prolyl oligopeptidase (POP) inhibitor identification via computational molecular designing approaches. **Bioinfo 2015**, Seoul National University, Korea; p 70, October 21-23, **2015**.
6. **Kumar R**, Son M, Lee Y, Bavi R, Park C, Arulalapperumal V, Lee KW. Development of 3D QSAR pharmacophore model for designing lead candidates of AKR1B10 inhibitors. **Bioinfo 2014** Seoul, Yonsei University, Korea; p 97, November12-14, **2014**.
7. **Kumar R**, Son M, Lee Y, Bavi R, Park C, Arulalapperumal V, Lee KW. Ligand- based pharmacophore modeling and supplementary approaches to

identify AKR1B10 inhibitors. **The 3rd International GNU Symposium on Agrobiotechnology 2014**; BNIT R&D Center, GNU, Jinju, Korea; p 95, September 21-23, 2014.

Reviewer for Refereed Journals

1. Nutrients (IF: 5.7)
2. Computers in Biology and Medicine (IF: 4.5)
3. Molecules (IF: 4.4)
4. Scientific Reports (IF: 4.3)
5. Life (IF: 3.8)
6. International Journal of Environmental Research and Public Health (IF: 3.3)
7. Journal of Receptors and Signal Transduction (IF: 2.1)
8. VirusDisease (IF: 1.2)

Academic Activities/Responsibilities

Teaching

B. Tech.

- Structural Biology (Lecture, Tutorial, Practical)
- Structural Bioinformatics (Lecture, Tutorial, Practical)
- Computer Aided Drug Design (Lecture, Tutorial, Practical)
- Biological Computation (Lecture, Tutorial, Practical)
- Introduction to Bioinformatics (Lecture, Tutorial, Practical)
- Computational Systems Biology (Lecture)
- Linux Lab (Practical)

M. Tech.

- Advanced Bioinformatics (Lecture, Practical)
- Advances in Computational Systems Biology (Lecture)

M. Sc.

- Bioinformatics (Lecture, Practical)

Research Guidance

- Guided 1 M.Sc. student in Biotechnology at JUIT, Wagnaghat, H.P., India.
- Guided 1 M.Tech. student in Biotechnology at JUIT, Wagnaghat, H.P., India.
- Guided 13 B. Tech. students for their final projects during 2019-2023.

Conferences/Workshops Organized

1. **Coordinator:** One week **DST-STUTI-ICT** sponsored workshop entitled “**A hands-on Training Program on Approaches for Screening and Characterization of Pre-clinical Drug Candidates**” hosted by Jaypee University of Information Technology, Wagnaghat, Solan (HP), India.
2. **Organizing member:** International virtual conference on “**Technologies for environmental sustainability and smart agriculture**”, 18-19th Sept, 2020 organized by Centre of excellence in sustainable technologies for rural development (CESTRD),

Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Wagnaghat, Solan (HP), India.

3. **Organizing member:** International virtual conference on “**International conference on Renewable Energy for Sustainable Environment**”, to be held in the month of Oct, **2021**, organized by Centre of excellence in sustainable technologies for rural development (CESTRD), Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Wagnaghat, Solan (HP), India.

Guest Lectures

1. **Special summer lecture** on the topic 'Computational Approaches to Identify Potential Drug Molecules' at the University of Illinois College of Medicine Rockford, USA.
2. **Seminar talk** on the topic “Managing Big Data from Large Scale Polymer Simulations using Martini Coarse Grained Modeling” at Department of Physics, **Gyeongsang National University**, South Korea on 7th July, 2022.
3. **Guest of Honor** at online workshop entitled “Basic of Bioinformatics-with research orientation towards drug and vaccines” organized by Institute of Biological Science, SAGE University, Indore (M.P.), India.
4. Delivered **expert session** on “An introduction to Computer-Aided Drug Design” held on 31st Oct, 2020 organized by Institute of Biological Science, SAGE University, Indore (M.P.), India.
5. Delivered **expert session** on “Computational Drug Repurposing for COVID-19 Treatment” under Faculty Development Program held on 15th May, 2021 organized by Institute of Biological Science, SAGE University, Indore (M.P.), India.

FDP/Conferences/Workshops/Webinars

1. Completed **short course** on ‘Machine Learning for Data Science using Python’, organized by Department of Computer Science and Engineering, National Institute of Technology (NIT), Warangal, India from May 16-31, 2023.
2. Completed AICTE Training And Learning (ATAL) Academy Blended/Hybrid **Faculty Development Programme (FDP)** on "Computational Biology in Therapeutics and Theranostics" from 2022-10-10 to 2022-10-15 and 2022-10-17 to 2022-10-21 at Indian Institute of Information Technology, Allahabad.
3. Completed one week AICTE Recognized **Faculty Development Programme (FDP)** on “NEP 2020 Implementation in Higher Education Institutes” organized by National Institute of Technical Teachers Training & Research (NITTTR) Chandigarh, India from 09/05/2022 to 13/05/2022.
4. Participated in the **one-day workshop** entitled “Environment and Sustainability” organized by Jaypee Institute of Information Technology, Noida and Jaypee University of Information Technology, Wagnaghat on 9 June 2022.
5. Participated in **National Science Day Symposium (NSDS 2022)** event organized by Jaypee University of Information Technology, Wagnaghat, Solan, HP, India in association with HIMCOSTE, Govt. of H.P. on February 28, 2022.

6. **Session chair** in virtual international conference on “Technological Intervention in Renewable Energy for Sustainable Environment (**RESE-2021**)” organized by Technology Incubation and Entrepreneurship Development (TIED) Cell and Centre of Excellence in Sustainable Technologies for Rural Development [CESTRD], Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology during November 24 & 25, 2021.
7. Participated in **webinar** “Attracting grants and funds for research” organized by WILEY, September 14, 2021.
8. Participated in **international webinar** “Clinical Bioinformatics: Bridging the Gateway to Precision Medicine” organized by Centre of Excellence in Health Care Technologies and Informatics (CEHTI), Department of Biotechnology and Bioinformatics, JUIT on January 12, 2021.
9. Participated in **international webinar** “Longitudinal Modeling of Alzheimer's Disease Using Machine Learning Methods” organized by Centre of Excellence in Health Care Technologies and Informatics (CEHTI), Department of Biotechnology and Bioinformatics, JUIT on December 07, 2020.
10. Participated in **international webinar** “Clinical Bioinformatics: Bridging the Gateway to Precision Medicine” organized by Centre of Excellence in Health Care Technologies and Informatics (CEHTI), Department of Biotechnology and Bioinformatics, JUIT on November 06, 2020.
11. Participated in **international webinar** “E-Waste and Health Care” organized by Centre of Excellence in Health Care Technologies and Informatics (CEHTI), Department of Biotechnology and Bioinformatics, JUIT on October 09, 2020.
12. Three days’ **workshop** on “Perception towards IPR” held on 10-12th Feb 2020 at Jaypee University of Information Technology, Wagnaghat, Solan (HP), India.

Memberships in Institute Activities & Development

- Board member of Centre of Excellence in Healthcare Technologies and Informatics (CEHTI) Department of Biotechnology and Bioinformatics, Jaypee University of Information Technology, Wagnaghat, Solan (HP), India.
- Member of the IQAC-Institutional Values & Best Practice Committee.
- Member of the Moodle Implementation Committee.
- Member of the University Level Committee.
- Member of faculty screening committee 2021.
- Faculty mentor for B. Tech- Bioinformatics 2nd and 4th year students
- Faculty mentor for M. Tech- Biotechnology 2nd year students
- Panel member for conducting Mock Interviews of final year B. Tech. students
- Member of the “Royal Society of Biotechnology and Biosciences”
- External Examiner, Shoolini University, India

Additional Qualification

- General Course on Intellectual Property, distant learning from WIPO Academy, Geneva, Switzerland (2013).

- National training program on “Bioinformatics: Methods, Tasks and Applications in Microbial Research” at National Bureau of Agriculturally important Microorganisms (NBAIM), Mau, India (2012).
- Certificate of Biotech Industrial Training Program (BITP) organized by Biotech Consortium India Limited (BCIL), New Delhi, India (2011).
- Bio-Business Management from Shoolini Institute of Life Sciences and Business Management (SILB), Solan, India (2008).
- Short course in Computer Hardware and maintenance from Govt. Polytechnic College for Women, Kandaghat, India (2008).

Declaration

I hereby declare that the above-mentioned information is correct up to my knowledge and I bear the responsibility for the correctness of the above-mentioned particulars.

Raj Kumar