

## BIOGRAPHICAL SKETCH

- 1. Name :** Rituraj Purohit
- 2. Designation:** Senior Principal Scientist
- 3. Department/Institute/University :** Department of Biotechnology, CSIR-Institute of Himalayan Bioresource Technology, Palampur, Himachal Pradesh -176061.  
Email; rituraj@ihbt.res.in

### 4. Education

S. No.	Institution Place	Degree Awarded	Field of Study
1.	BR Nahata College of Pharmacy - [BRNCP], Mandsaur	B.Pharmacy	Pharmaceutical Sciences
2.	Indian Institute Of Information Technology, Allahabad India	M.Tech	Bioinformatics
3.	Vellore Institute of Technology,University, Vellore, India.	Ph.D	Bioinformatics

### 5. Position

S. No.	Institution Place	Position	From (Date)	To (date)
1.	Department of Biotechnology, CSIR-Institute of Himalayan Bioresource Technology, Palampur (H.P.) India	Senior Principal Scientist	2023	Till Date
2.	Department of Biotechnology, CSIR-Institute of Himalayan Bioresource Technology, Palampur (H.P.) India	Principal Scientist	2018	2023
3.	Department of Biotechnology, CSIR-Institute of Himalayan Bioresource Technology, Palampur (H.P.) India	Senior Scientist	2014	2018
4.	School of Bio Sciences and Technology, Vellore Institute of Technology,University, Vellore, India.	Associate Professor	2013	2014
5.	Italian Institute for Genomic Medicine, Torino, Italy (Formerly known as; Human Genetics Foundation (HuGeF))	Postdoctoral Researcher	2012	2013
6.	School of Bio Sciences and Technology, Vellore Institute of Technology,University, Vellore, India.	Assistant Professor	2007	2012

### 6. Key Publications:

- 1) Identification and evaluation of olefinated benzosuberene analogue as a phosphodiesterase-4D inhibitor with efficacy in a zebrafish larva model of pentylenetetrazole-induced seizures.  
Bhanu Sharma, Shubham Nilkanth Rahmatkar, Ashish Kumar, Pralay Das, Damanpreet Singh\* and Rituraj Purohit\*  
Chemical Engineering Journal 507 (2025) 160272
- 2) A comparative study on inclusion complex formation between formononetin and  $\beta$ -cyclodextrin derivatives through multiscale classical and umbrella sampling simulations.  
Vijay Kumar Bhardwaj and Rituraj Purohit\*  
Carbohydrate Polymers 310 (2023) 120729
- 3) Mechanistic behavior and subtle key events during DNA clamp opening and closing in T4 bacteriophage  
Vijay Kumar Bhardwaj, Aaron Oakley and Rituraj Purohit\*  
International Journal of Biological Macromolecules (2022) 208: 11-19
- 4) Identification of 11 $\beta$ -HSD1 inhibitors through enhanced sampling methods.  
Rahul Singh, Vijay Kumar Bhardwaj, Pralay Das, and Rituraj Purohit\*  
Chemical Communications (2022) DOI: 10.1039/D1CC06894F

- 5) Integrating microsecond timescale classical and biased molecular dynamics simulations to screen potential molecules for BRD4-BD1.  
Vijay Kumar Bhardwaj, Pralay Das and Rituraj Purohit\*  
Chaos, Solitons and Fractals (2023) 167:113061
- 6) Taming the ringmaster of the genome (PCNA): Phytomolecules for anticancer therapy against a potential non-oncogenic target.  
Vijay Kumar Bhardwaj and Rituraj Purohit\*  
Journal of Molecular Liquids (2021) 337:116437.
- 7) Himalayan bioactive molecules as potential entry inhibitors for the human immunodeficiency virus.  
Vijay Kumar Bhardwaj, Rituraj Purohit\* and Sanjay Kumar  
Food Chemistry (2021) 347:128932
- 8) Explicit-solvent molecular dynamics simulations revealed conformational regain and aggregation inhibition of I113T SOD1 by Himalayan bioactive molecules.  
Sachin Kumar, Vijay Kumar Bhardwaj, Rahul Singh and Rituraj Purohit\*  
Journal of Molecular Liquids (2021) 339: 116798
- 9) Structural based study to identify new potential inhibitors for Dual Specificity Tyrosine- Phosphorylation-Regulated Kinase..  
Vijay Kumar Bhardwaj, Rahul Singh, Jatin Sharma, Pralay Das and Rituraj Purohit\*  
Computer Methods and Programs in Biomedicine. (2020) 194:105494
- 10) Benchmarking the ability of novel compounds to inhibit SARS-CoV-2 main protease using Steered molecular dynamics simulations.  
Rahul Singh, Vijay Kumar Bhardwaj, Pralay Das, Dhananjay Bhattacharjee, Grigory V. Zyryanov and Rituraj Purohit\*  
Computers in Biology and Medicine (2022) 146: 105572
- 11) A new insight into protein-protein interactions and the effect of conformational alterations in PCNA  
Vijay Kumar Bhardwaj and Rituraj Purohit\*  
International Journal of Biological Macromolecules (2020) 148:999-1009
- 12) Use of long term Molecular Dynamics Simulation in predicting cancer associated SNPs.  
Ambuj Kumar and Rituraj Purohit\*  
PLOS Computational Biology (2014) 10(4): e1003318

***Total number of refereed journals – 150 (125 as corresponding author)***

*Last updated on April 2025*