

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) Refining the Trapping of Therapeutic Agent Silybin A in Functionalized β - and γ -Cyclodextrin Cavitands for Improved Supramolecular Complexation.
Pramod Kumar and Rituraj Purohit*
Journal of Chemical Information and Modeling (2025) doi; 10.1021/acs.jcim.5c00625
- 2) 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
- 3) A comparative study on inclusion complex formation between formononetin and β -cyclodextrin derivatives through multiscale classical and umbrella sampling simulations.
Vijay Kumar Bhardwaj and Rituraj Purohit*
Carbohydrate Polymers 310 (2023) 120729
- 4) 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

- 5) Identification of 11 β -HSD1 inhibitors through enhanced sampling methods.
Rahul Singh, Vijay Kumar Bhardwaj, Pralay Das, and Rituraj Purohit*
Chemical Communications (2022) DOI: 10.1039/D1CC06894F
- 6) 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
- 7) 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.
- 8) 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
- 9) 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
- 10) 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
- 11) 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
- 12) 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
- 13) 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 – 151 (126 as corresponding author)