

BIOGRAPHICAL SKETCH

1. Name : Rituraj Purohit

2. Designation: Scientist-F

3. Department/Institute/University : Department of Biotechnology, CSIR-Institute of Himalayan Bioresource Technology, Palampur, Himachal Pradesh -176061.

Email; rituraj.purohit@csir.res.in;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	Scientist-F	2023	Till Date
2.	Department of Biotechnology, CSIR-Institute of Himalayan Bioresource Technology, Palampur (H.P.) India	Scientist-E	2018	2023
3.	Department of Biotechnology, CSIR-Institute of Himalayan Bioresource Technology, Palampur (H.P.) India	Scientist-D	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) Expanding the therapeutic landscape of PDE10A inhibition through alchemical absolute binding free energy calculations and in-vitro evaluation.
Bhanu Sharma, Rahul Singh, Ashish Kumar, Pralay Das and **Rituraj Purohit***
Protein Science (2026) 35 (2), e70472
- 2) 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
- 3) 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

- 4) Highly robust quantum mechanics and umbrella sampling studies on inclusion complexes of curcumin and β -cyclodextrin.
Pramod Kumar, Vijay Kumar Bhardwaj and **Rituraj Purohit***
Carbohydrate Polymers (2024) 323 :121432
- 5) 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
- 6) 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
- 7) 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
- 8) 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
- 9) 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.
- 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) 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 – 160 (130 as corresponding author)

Last updated on June 2026