

# Shailya Verma

## Research Scholar (Int. Ph.D)



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### Work Experience / Internship

**National Centre for Biological Sciences |**  
**Research Scholar | Integrated PhD | Aug 2018-**  
**Present**



#### Key Research Areas

- Understanding the sequence and structure of various Toll/interleukin-1 (IL-1) receptor (TIR) domains containing proteins.
- Studying the structural effect of mutations with the help of modeling, molecular dynamics simulation, protein residue network analysis.
- Structure based drug designing through virtual screening pipeline and in vitro experimental validation.

**Bhabha Atomic Research Centre |**  
**(SRFP) INSA-IASc-NASI | June 2017- July**



#### Key Research Areas

- Structure based drug design using Ribosome as a target.

**ANDC, Delhi University | Summer Elite Project |**  
**June 2016- July 2016**



#### Key Research Areas

- Studied Interaction of Plasmodium vivax Duffy Binding Protein (PvDBP) with its host receptors the Duffy Antigen (Fy) on RBC Surface using Bioinformatics Tools



### Education

- Integrated PhD, Biological Sciences  
NCBS - TIFR |2018 - Present
- B.Sc. (Hons.), Biomedical Sciences  
ANDC, Delhi University| 2015 - 2018
- Sunbeam School  
CBSE| 2009-2014



### Awards and Achievements

- Selected as **speaker** for NCBS annual talk 2023 (Patterns of Biology)
- Selected for European Conference on Computational Biology held in Barcelona, Spain 2022 with the prestigious **DBT-CTEP travel grant**.
- **Best poster award** in NCBS annual talk 2022 (Facets of Biology).
- **Volunteered for COVID-19** testing at inStem -NCBS testing facility (2020).
- Secured **AIR 82** in **CSIR-UGC-NET**, 2019.
- Granted **DAE - TIFR GS fellowship** for pursuing Integrated PhD ( 2018- 2024).
- Selected for **Ideathon, Nobel Prize Series** in Ahmedabad, Gujarat - **2017**



### Language

- English
- Hindi



## Research Summary

- As a graduate scholar my research focus is to unravel some unanswered questions of Toll-like receptor (TLR) pathways. In my PhD journey so far I have worked on sequence searches to look for evolutionary divergence of TLR adaptors among orthologues. I was able to map the changes at protein structural domains and residue level. I have also investigated the effect of selection pressure at protein sequence levels.
- In addition, I have experience with protein modeling, molecular docking, virtual screening, molecular dynamics. Using these approaches, I have found small molecule inhibitors for TLR4 pathway, to abrogate downstream signalling in diseased conditions. Using my computational study results further I was able to purify the protein to validate through in vitro experiments.
- In future I aim to learn Artificial intelligence and machine learning for predicting drug like molecules.



## Publications

- **Verma S**, Reddy P, Sowdhamini R. Integrated approaches for the recognition of small molecule inhibitors for Toll-like receptor 4. Comput Struct Biotechnol J. 2023 Jul 22;21:3680-3689. doi: 10.1016/j.csbj.2023.07.026. PMID: 37576745; PMCID: PMC10412839.
- **Shailya Verma**, Revathy Menon, Ramanathan Sowdhamini. Structural insights into the role of deleterious mutations at the dimeric interface of TRAM protein. Authorea. May 29, 2023. DOI: [10.22541/au.168534396.69412137/v1](https://doi.org/10.22541/au.168534396.69412137/v1) (Submitted and under review - PROTEINS: Structure Function, and Bioinformatics)
- Bhattacharyya T, Ghosh A, **Verma S**, Raghu P, Sowdhamini R. Structural rationale to understand the effect of disease-associated mutations on Myotubularin. Curr Res Struct Biol. 2023 Mar 22;5:100100. doi: 10.1016/j.crstbi.2023.100100. PMID: 37101954; PMCID: PMC10123148.
- **Verma S**, Sowdhamini R. A genome-wide search of Toll/Interleukin-1 receptor (TIR) domain-containing adapter molecule (TICAM) and their evolutionary divergence from other TIR domain containing proteins. Biol Direct. 2022 Sep 2;17(1):24. doi: 10.1186/s13062-022-00335-9. PMID: 36056415; PMCID: PMC9440496.



## Skills and Competency

- **Bioinformatics**
  - Phylogenetics, Sequence based evolutionary analysis, Mutational studies, Protein Modeling, Molecular Docking, Virtual screening, Molecular Dynamics simulations, Protein residue network analysis
- **Biochemistry**
  - Cloning, Protein expression and purification, Western blotting, Chromatography, Site directed Mutagenesis, Isothermal Calorimetry
- **Cell Biology**
  - Tissue culture handling, Cell based reported assay, Cell viability assay, Polymerase chain reaction