Dr Harvinder Singh (PhD, MSc)

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Summary

I, Dr Harvinder Singh, a postgraduate microbiologist, hold a PhD in **Computer Aided Drug-designing and Discovery for Drug-resistant epilepsy** (26.07.2024) from the Postgraduate Institute of Medical Education and Research, Chandigarh, India. My thesis work was focused on the drug-discovery program for the neuro-degenerative disorder drug-resistant epilepsy. The thesis work consists of three platforms ***in-silico*** *(*virtual screening, molecular dynamics simulations {gmx_qk}, and free-energy calculations*),* ***in-vitro*** *(*validation of lead compounds in wet lab*) and* ***in-vivo*** *(*Assessment of pharmacological activity of selected compound in drug-resistant epilepsy rodent model *).*

In the last **five** years, I have completed two **Johns Hopkins University** specialisations in **Data Science and Genomic Data Science.**

I've published several papers in the last five years, including **two** systematic reviews and meta-analyses, **twelve** original research articles (list enclosed), **two** book chapters, an editorial, an R package and LINUX-based gmx_qk (JCIM-ACS).

Experience

Research Associate (PGIMER, Chandigarh)

Dept. of Translational and Regenerative Medicine, PGIMER, Chandigarh

Jan 2024 – Nov 2025

Research Scholar (PhD Pharmacology)

Dept. of Pharmacology, **Post Graduate Institute of Medical Education and Research, Chandigarh**

July 2019 – December 2024

The thesis entitled "***Evaluation of the pharmacological activity of new chemical entity and existing hit or lead compound via targeting the long term potentiation pathway in the experimental models of drug-resistant epilepsy"*** involved all preclinical platforms i.e., *in-silico, in-vitro and in-vivo*. I have learned about advancements in computer-aided drug design and discovery, i.e., molecular docking, virtual screening, QSAR, Molecular dynamics and Meta-dynamics simulations, and free-energy calculations. During this period I have contributed to computational as well as *in-vivo studies (animal models of neurodegenerative disorders)* and published in reputed peer-reviewed journals i.e., **JBSD, ACS JCIM** (IF 5.8), and **ACS Pharmacology and Translational Science** (**IF 6.0**).

Publications (Best 10)

1. Badal R, Kaur B, Singh H, Sharma P, Yadav P, Mahapatra A, et al. Saraswata Ghrita mitigates $AlCl_3$-and D-galactose–induced cognitive deficits in a murine Alzheimer's-like model: In silico and in vivo insights. Brain Res Bull. 2026;2026:111742.
2. Gupta T, Devi V, Rao A, Bharti R, Singh H, Kumar M, et al. Molecular forensics: RNA degradation as a marker for postmortem interval determination. Int J Legal Med. 2026:1-13.
3. Bhat S, Basak P, Verma S, Siddiqui K, Dutta P, Das L, et al. Type 2 diabetes compromises SARS-CoV-2-specific immunological memory following ChAdOx1 nCoV-19 vaccination. Vaccine. 2025;62:127604.
4. Jain A, Dhir N, Prabha PK, Raja A, Sharma AR, Kaundal T, et al. Restoring brain function in autism: GSK3β inhibition by 6-bromoindirubin-3′-oxime reverses valproic acid-induced neuropathology. ACS Chem Neurosci. 2025;16(13):2395-2419.
5. **Singh H**, Raja A, Chauhan A, Jain A, Prakash A, Bhatia A, Avti P, Medhi B. Unlocking the Therapeutic Potential: Sitagliptin's Multifaceted Approach in Drug-Resistant Epilepsy through a Novel Mechanism Inhibiting Protein Kinase C-γ and a Long-Term Potentiation Pathway. ACS Pharmacology & Translational Science. 2024 May 13. (https://doi.org/10.1021/acsptsci.4c00073)
6. **Singh H,** Raja A, Prakash A, Medhi B. Gmx_qk: An Automated Protein/Protein–Ligand Complex Simulation Workflow Bridged to MM/PBSA, Based on Gromacs and Zenity-

Dependent GUI for Beginners in MD Simulation Study. Journal of Chemical Information and Modeling. 2023 Apr 20. (https://doi.org/10.1021/acs.jcim.3c00341)

7. **Singh H**, Raja A, Shekhar N, Chauhan A, Prakash A, Avti P, Medhi B. Computational attributes of protein kinase-C gamma C2-domain & virtual screening for small molecules: elucidation from meta-dynamics simulations & free-energy calculations. Journal of Biomolecular Structure and Dynamics. 2022 May 14:1-2. (https://doi.org/10.1080/07391102.2022.2077447)
8. Kaur B, Singh H, Choudhary G, Prakash A, Medhi B, Chatterjee D, Saini UC, Kaur J, Verma I, Sharma S. Natural angiotensin II type 1 receptor inhibitors: Virtual screening and in vitro evaluation of beta-1, 2, 3, 4, 6-penta-O-galloyl-d-glucopyranose, icarrin, and sesamin for osteoarthritis therapy. International Journal of Biological Macromolecules. 2025 Mar 25:142184. (http://dx.doi.org/10.1016/j.ijbiomac.2025.142184)
9. Raja A, Shekhar N, **Singh H**, Prakash A, Medhi B. In-silico discovery of dual active molecule to restore synaptic wiring against autism spectrum disorder via HDAC2 and H3R inhibition. Plos one. 2022 Jul 25;17(7):e0268139.
10. Kaur G, Prajapat M, **Singh H**, Sarma P, Bhadada SK, Shekhar N, Sharma S, Sinha S, Kumar S, Prakash A, Medhi B. Investigating the novel-binding site of RPA2 on Menin and predicting the effect of point mutation of Menin through protein–protein interactions. Scientific Reports. 2023 Jun 8;13(1):9337.
11. Kumar S, **Singh H**, Prajapat M, Sarma P, Bhattacharyya A, Kaur H, Kaur G, Shekhar N, Kaushal K, Kumari K, Bansal S. Structural-Based Virtual Screening of FDA-Approved Drugs Repository for NSP16 Inhibitors, Essential for SARS-COV-2 Invasion Into Host Cells: Elucidation From MM/PBSA Calculation. Bioinformatics and Biology Insights. 2023 Jul;17:11779322231171777.
12. Chauhan A, Singh J, Sangwan N, **Singh H**, Prakash A, Medhi B, Avti PK. Designing the 5HT2BR structure and its modulation as a therapeutic target for repurposing approach in Drug-resistant epilepsy. Epilepsy Research. 2023 May 30:107168.
13. Prajapat M, **Singh H**, Chaudhary G, et al. A Novel Inhibitor of DKK1/LRP6 Interactions Against the Alzheimer Disease: An Insilco Approach. Bioinformatics and Biology Insights. 2023;17. doi:10.1177/11779322231183762
14. Shekhar N, Sarma P, Prajapat M, Avti P, Kaur H, Raja A, **Singh H**, Bhattacharya A, Sharma S, Kumar S, Prakash A. In silico structure-based repositioning of approved drugs for spike glycoprotein S2 domain fusion peptide of SARS-CoV-2: rationale from molecular dynamics and binding free energy calculations. Msystems. 2020 Sep 22;5(5):e00382-20.

15. Prakash A, **Singh H**, Sarma P, Bhattacharyya A, Dhibar DP, Balaini N, Shree R, Goyal M, Modi M, Medhi B. nCoV-2019 infection induced neurological outcome and manifestation, linking its historical ancestor SARS-CoV and MERS-CoV: a systematic review and meta-analysis. Scientific reports. 2021 Jun 18;11(1):1-5.

Book chapters and reviews

1. Singh H, Singh P, Chaudhary G, Singh H. Protein Structure Modeling and Refinement. (http://dx.doi.org/10.1016/B978-0-323-95502-7.00193-7)
2. Kaur G, Singh RS, Singh A, **Singh H,** Sinha S, Medhi B. Translational Epidemiology in Cancer Research: The Less Travelled Path. InBiomedical Translational Research: From Disease Diagnosis to Treatment 2022 Jun 15 (pp. 349-366). Singapore: Springer Nature Singapore.
3. Raja A, Mahendiratta S, **Singh H**, Shekhar N, Prakash A, Medhi B. Nanoparticles in Chronic Respiratory Diseases. InAdvanced Drug Delivery Strategies for Targeting Chronic Inflammatory Lung Diseases 2022 Mar 24 (pp. 143-170). Singapore: Springer Singapore.
4. Bhandari PR. Textbook of pharmacology. Thieme; 2022 Sep 22. (**CNS Stimulants and Drugs of Abuse)**
5. Kumar S, Sarma P, Kaur H, Prajapat M, Bhattacharyya A, Avti P, Sehkhar N, Kaur H, Bansal S, Mahendiratta S, Mahalmani VM, **Singh H**. Clinically relevant cell culture models and their significance in isolation, pathogenesis, vaccine development, repurposing and screening of new drugs for SARS-CoV-2: a systematic review. Tissue and Cell. 2021 Jun 1;70:101497.
6. Singh H, Choudhary G, Siddiqui H, Singh P, Singh L, Singh S, et al. AI in biomolecular structural data analysis. Academic Press; 2026.

Work Accomplishments

Major Challenges:

- Starting from scratch in identifying an inhibitor for the Protein Kinase C Gamma (PKCγ) C2 domain was one of the most challenging tasks. There was no binding site information available, except for the Pyridoxal and Calcium co-factor binding sites.

- Another significant challenge arose with MM/PBSA and binding free energy calculations, as the available tools were proprietary and prohibitively expensive, such as Schrödinger's Maestro suite.
- Access to computational resources like high-performance computing (HPC) was also limited.

Overcome the challenges:

- The structural characteristics of the PKCγ-C2 domain were analyzed by comparing it with other isoforms, which led to the identification of a specific calcium-binding cleft with unique residues for specificity.
- To address the second challenge, I leveraged the flexibility of GROMACS and bash scripting to develop **gmx_qk**, a completely free workflow for energy calculations from MD trajectories, similar to the Maestro suite. This solution significantly improved reproducibility and allowed for energy decomposition analysis, determining the contribution of individual residues to the binding free energy.
- I managed the computational resources on a local system equipped with a single GPU (24GB) and CPU (32GB RAM).

Conferences and Training

- **7th National Workshop on Pharmacogenomics-2024** Demonstrated the analysis of Sanger sequencing data using R.
- **The 22nd International Conference on Bioinformatics (InCoB) – 12-15th November, 2023 :** Oral presentation on "Gmx_qk: An Automated Protein/Protein–Ligand Complex Simulation Workflow Bridged to MM/PBSA, Based on Gromacs and Zenity-Dependent GUI for Beginners in MD Simulation Study"
- **Insights into Insilico Techniques in Drug Discovery: A Hands-On Workshop (organized)** on 19th June 2023.
- **Computational Workshop on Genomics, Proteomics and Metagenomics (CWGPM – 2022)** DBT-sponsored instructional workshop organised by **Bioinformatics Centre, CSIR-IGIB, New Delhi**. A hands-on session for genomics data analysis and interpretation.
- **1st International Agriculture Conference GIRISDA-2022, June 2022 "Warabandi, A R package to generate roster of turn for weekdays"**

- **International Conference on Drug Discovery 2022 (**Presented a poster on "Gmx_qk: An Automated Protein/Protein–Ligand Complex Simulation Workflow Bridged to MM/PBSA, Based on Gromacs and Zenity-Dependent GUI for Beginners in MD Simulation Study")
- **11th (Nort zone) "CME on Pharmacovigilance / Materiovigilance and coordinators Meeting" 2023, (Organizer)**
- **6th Advanced Training Program in Experimental Behavioural Neurosciences, 2023 (Organizer)**
- **5th National Workshop on "PHARMACOGENOMICS: BASICS TO ADVANCED", 2022** (Demonstrated **"SNP and RNAseq analysis")**
- **National Hands-on Workshop on "Applications of Flow Cytometry In Pharmacology and Drug Discovery", 2019 (**Participated)
- **Indian Journal of Pharmacology (IJP) – British Journal of Pharmacology (BJP) Joint Symposium, 2019 (**Participated**)**

Education

1. **PhD Pharmacology** **(Jul 2019 – December 2023)**
   Dept. of Pharmacology, **Post Graduate Institute of Medical Education and Research, Chandigarh**
2. **Specialization, Genomic Data Science** **Mar 2021 - Sep 2021**
   (The Johns Hopkins University)

3. **Specialization, Data Science** **Mar 2020 - Nov 2020**
   (The Johns Hopkins University)
4. **Pre PhD, MICROBIOLOGY** **(2017 – 2018)**
   (Guru Nanak Dev University, Amritsar)

   - Research Methodology: Experiment designing and statistical analysis in basic research and surveys
   - Molecular and Analytical Techniques: Gas-Chromatography-Mass Spectrometry (GCMS), Microbial culture techniques and staining, DNA-RNA extraction as well sequencing.
   - Disaster Management: Precautions and lifesaving hacks while working in the laboratory.

5. **M.Sc., Microbiology (Vocational)** **(2015 – 2017)**
   (M.D.(PG) College, Sri Ganganagar)
6. **B.Sc., Microbiology (Vocational)** **(2012 – 2015)**
   M.D. (PG) College, Sri Ganganagar, Rajasthan

Licenses & Certifications

- **Certified Instructor – Data Carpentries- 2024**
- **JUNIOR FOOD ANALYST - Food Safety And Standards Authority Of India (FSSAI)**
- **Junior research fellowship** - Council of Scientific and Industrial Research -2018
- **GATE** - IIT Guwahati-2018
- **LECTURESHIP/ ASSISTANT PROFESSORSHIP** - Indian Council of Agricultural Research-2018
- **Junior research fellowship** – Indian Council of Medical Research-2020

Skills

- Wet lab skills:
  - **Animal handling (rats: Neurodegenerative disease models)**
  - Enzyme assay and microbial culture techniques
  - Molecular Techniques: **DNA-RNA extraction as well as sequencing**
- Molecular docking and virtual screening using **AutoDock** Vina
- Molecular modelling and Simulations using **Schrodinger** as well as **Gromacs** (Gmx_qk)
- Programming languages **R, Python and BASH, OS-LINUX**
- Molecular mechanics and quantum mechanics free energy calculations using **MM/PBSA and MM/GBSA**

  Biased molecular simulations using **PLUMED**
- **Data analysis and machine learning**
  - Experiments Designing
  - **Markdown and code management**
  - **NGS data analysis (SNPs, and Variations)**
  - **RNA-Seq analysis pipeline using the command line as well as bio-conductor**
  - **Basic statistics**, exploratory data analysis and **Machine Learning**

Honours & Awards

1. **Young Scientist Travel Award (DST-SERB, New Delhi) -** 22nd International Conference on Bioinformatics **(InCoB-2023) Brisbane (Australia),** Oral presentation on "An Automated Protein/Protein–Ligand Complex Simulation Workflow Bridged to MM/PBSA, Based on Gromacs and Zenity-Dependent GUI for Beginners in MD Simulation Study"
2. **Best Poster Presentation** - 1st International Agriculture Conference **GIRISDA-2022** June 2022 "Warabandi, A R package to generate roster of turn for weekdays"