# ISHWAR CHANDRA, M.Pharm., M.Phil.

Address: C/O Mr. Sikamani, 3515, Karpaga Vinayagar Nagar, 1st Main Road
Burma Colony, Sekkalaikottai, Karaikudi, 630002, Tamil Nadu, India
Mobile: +918469611421 Email id: auishwar@gmail.com

**Objective:** An energetic, versatile and quick learning individual with a wide and intense enthusiasm for the discovery of new innovative drugs and to develop new aptitudes to solve new challenges.

## Experience

Employer's Name : Structural Bioinformatics and CADD Lab, under Prof. Sanjeev Kumar Singh at Department of Bioinformatics, Alagappa University, Karaikudi.
Duration : January 04, 2016 to November 15, 2022.
Post Held : **Research Assistant**.
Job Description : Literature search to find drug targets and existing therapies, to implement computer aided drug design for identifying novel inhibitors of the disease through high throughput virtual screening, docking and molecular dynamics studies.

Employer's Name : Infodesk India Private Limited. Vadodara, Gujarat.
Duration : September 25, 2014 to November 30, 2015.
Post Held : **Research Analyst**.
Job Description : Involve in mapping of pharmaceutical details like drug names, mechanism of action, indications, company, patent information, clinical trial information from different resources for developing Infodesk Pharmaintelligence: The Premier Pharmaceutical Information Platform.

Employer's Name : National Institute of Virology, Pune.
Duration : January 27, 2012 to March 31, 2014.
Post Held : **Senior Research Fellow**.
Job Description : Computer aided drug design by using pharmacophore and docking studies of human influenza proteins. Assisted in teaching bioinformatics classes of M.Sc Virology at NIV,Pune.

Employer's Name : TRR College of Pharmacy Patancheru, Hyderabad.
Duration : 14 July 2009 to 24 January 2012.
Post Held : **Assistant Professor**.
Job Description : Lectureship; conducting theory and practical classes. Assisting in college administration.

Employer's Name : Bhawani Medical Hall, P.O. Bahera, District Darbhanga, Bihar.
Duration : 1 August 2005 to 28 February 2007.
Post Held : **Pharmacist**.
Job Description : Dispensed medicines as prescribed on the doctor's prescription.
Stock management and store keeping.

## Skills

BIOINFORMATICS TOOLS

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|---|---|
| Docking Tools | GOLD, GLIDE, Sybyl, Auto-dock, Argus Lab |
| Molecular Dynamics Tools | Desmond, GROMACS |
| Molecular Visualization Software | Discovery Studio Visualiser,Pymol,SPDBV |
| Molecular Modelling Tools | Chemsketch,Chemdraw, Modeller |
| Alignment Tools | Clustal X,ClustalW, Multalign. |
| Sequence Analysis Tool | EMBOSS, BLAST |

**Education:**

| Examination Passed | Year of Passing | Institute/ University | CGPA % |
|---|---|---|---|
| Ph.D. (Bioinformatics) Thesis Submitted | 2022 | Alagappa University Karaikudi (Tamil Nadu) | -- |
| M.Phil Basic Medical Science (Pharmacoinformatics) | 2014 | School of Basic Medical Science, Savitribai Phule Pune University (Maharashtra) | A |
| M.Pharm Pharmacoinformatics | 2009 | School of Chemical & Biotechnology SASTRA University, Thanjavur (Tamil Nadu) | 7.77/10 |
| B.Pharm | 2005 | Kanak Manjari Institute of Pharmaceutical Sciences, Rourkela Sambalpur University (Odisha) | 67.3 |

**Publications**

***Research Articles***

- **Chandra, I.**, Prabhu, SV., Nayak, C., Singh, SK*. (2021). E-pharmacophore based screening to identify potential HIV-1 gp120 and CD4 interaction blockers for wild and mutant types. SAR and QSAR in Environmental Research. Apr 10:1-25. DOI: https://doi.org/10.1080/1062936X.2021.1901310
- Nayak, C., **Chandra, I.**, Singh, SK*. (2019). An in silico pharmacological approach toward the discovery of potent inhibitors to combat drug resistance HIV-1 protease variants. Journal of cellular biochemistry. Jun;120(6):9063-81. DOI: https://doi.org/10.1002/jcb.28181
- **Chandra, I**., Behera, AK., & Cherian, SS*. (2017). Identification of Potential Inhibitors against the Human Influenza A Virus Targeting the CPSF30 and RNA Binding Domains of the NS1 Protein: An E-Pharmacophore approach. Indian Journal of Pharmaceutical Education and Research, 51(1), 25-33. DOI: https://doi.org/10.5530/ijper.51.1.5
- Behera, AK., **Chandra, I**., & Cherian, SS*. (2016). Molecular dynamics simulation of the effects of single (S221P) and double (S221P and K216E) mutations in the hemagglutinin protein of influenza A H5N1 virus: a study on host receptor specificity. Journal of Biomolecular Structure and Dynamics, 34(9), 2054-2067. DOI: https://doi.org/10.1080/07391102.2015.1106341

***Review Articles***

- Selvaraj, C., **Chandra, I.**, Singh, SK*. (2021). Artificial Intelligence and Machine learning approaches for drug design: Challenges and Opportunities for the pharmaceutical industries. Molecular Diversity, Oct 23:1-21. DOI: https://doi.org/10.1007/s11030-021-10326-z
- Panwar, U., **Chandra, I.**, Selvaraj, C., Singh, SK*. (2019). Current Computational Approaches for the Development of Anti-HIV Inhibitors: An Overview. Current pharmaceutical design. Sep 1;25(31):3390-405. DOI: https://doi.org/10.2174/1381612825666190911160244

***Book Chapters***

- **Chandra, I.**, Nayak, C., Singh, SK*. (2021). Predicting Protein Folding and Protein Stability by Molecular Dynamics Simulations for Computational Drug Discovery. In Innovations and Implementations of Computer Aided Drug Discovery Strategies in Rational Drug Design (pp. 153-177). Springer, Singapore. DOI: https://doi.org/10.1007/978-981-15-8936-2_7
- Nayak, C., **Chandra, I.**, Singh, P., Singh, SK*. (2018) Omics-Based Nanomedicine. In Synthetic Biology (pp. 227-248). Springer, Singapore. DOI: https://doi.org/10.1007/978-981-10-8693-9_12
- Suryanarayanan, V., Panwar, U., **Chandra, I**., Singh SK*. (2018). De Novo Design of Ligands Using Computational Methods. Mohini Gore and Umesh B. Jagtap (Eds.), Computational Drug Discovery and Design, Methods in Molecular Biology, Vol. 1762 DOI: https://doi.org/10.1007/978-1-4939-7756-7_5

**Poster presentations**

- Presented poster at 1st International Conference on Recent Trends in Structural Bioinformatics and Computer Aided Drug Designing 2019 titled “Structure based screening ofAnti-HIV-1 Inhibitors by targeting V3 Loop in the envelope protein gp120” Organized by Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India, dated 11-13 December, 2019.
- Presented poster at 3rd International Science Symposium on HIV and Infectious Diseases 2019 titled “Unraveling Novel HIV-1 gp41 Inhibitors Using In-silico Approaches” Organized by Sri Ramchandra Institute of Higher Education and Research (SRIHER) and YRG Care, India at Porur, Chennai, dated 12-14 October, 2019. Published in BMC Infectious Diseases, Abstract-260. DOI: https://doi.org/10.1186/s12879-020-05038-y
- Presented poster at 11th National Symposium cum workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Designing 2019 titled “Identification of Novel HIV-1 Entry Inhibitors Using In-Silico Approaches” Organized by Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India, dated 12-15 February, 2019.
- Presented poster at 10th National Symposium cum workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Designing 2018 titled “Computational Approach for the Identification of Potential CD4-Mimetic HIV-1 Entry Inhibitors” organized by Organized by Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India.
- Presented poster at 9th National Symposium cum workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Designing 2017 titled “E-Pharmacophore Based Design of Novel Protease Inhibitors for HIV-1” organized by Organized by Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India.
- Poster presentation at Recent Advances on Computational Drug Design 2013 titled “E-Pharmacophore Mapping and Docking study of NS1 Protein of Human Influenza A Viruses” at IISc, Bangalore organized by IISc and Schrodinger.
- Presented poster at Silver Jubilee Bioinformatics Conference 2012 titled “Investigating NS1 Protein as a Novel Drug Target for Human Influenza A Viruses” organized by Department of Bioinformatics, University of Pune.
- Presented poster at Raman Memorial Conference 2012 titled “Investigating Influenza Neuraminidase Inhibitor Analogs for Finding Potential Drug Candidates: A Bioinformatics Approach” organized by Department of Physics, University of Pune.

**Personal Data**

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| **Father’s name** | Shri Bhola Prasad Dutt |
| **Date of Birth** | 25-05-1983 |
| **Marital Status** | Married |
| **Nationality** | Indian |
| **Registration** | Registerd Pharmacist at Jharkhand State Pharmacy Council, Ranchi, Registration No. 00381<br>Life Member at Bioinformatics and Drug Discovery Society, Karaikudi. Membership No. BIDDS17-47 |
| **Permanent Address** | Sector 2A, Qtr. No. 2-006, Bokaro Steel City,<br>Bokaro – 827001, Jharkhand, India |

**Declaration**

I vouch the authenticity of the above-mentioned information to the best of my knowledge and belief.

Ishwar Chandra