**Ashish Shelar, Ph.D**

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A dedicated and highly knowledgeable research scientist and bioinformatician specializing in biological sciences with extensiveexperience in Spatial Multi-omic algorithm design, data analysis and pipeline optimization. Excels at setting up and maintaining mass cytometry , Imaging Mass Cytometry and Spatial Genomic data analysis pipelines across multiple projects in inter-disciplinary environments. Collaborated with a team of cancer biologists and doctors (physician scientists) at Yale towards setting up custom analytical bioinformatics tools. Proven track record in the field of computational biology evidenced by research articles in high-impact scientific journals.

**Specialization Bioinformatics |Spatial Multi Omics| NGS data analysis** **| Algorithm Development | Machine Learning |Manuscript review and management**

**Research Experience**

**Bioinformatics Research Scientist, Yale Center for Genome Analysis** (2021 - Present)

* + - Designated as the primary point of contact for multiple principal investigators (PIs), providing expertise in project design and bioinformatics analysis
		- Acted as primary lead developer for implementation and maintenance of analysis pipelines for CyToF and Imaging Mass Cytometry (IMC) data analysis, ensuring reproducibility and efficiency
		- Working as the principal bioinformatics scientist to communicate with experimentalists in developing cutting edge spatial genomic technology pipelines (10X Xenium, Bruker CosMx, )
		- Developed and deployed customized data analysis and visualization techniques, enhancing insights from various genomic sequencing technologies

**Post-Doctoral Research Associate** (2019 - 2021)

Title Understanding neuronal communication in C. elegans using confocal imaging and neurotransmitter G-protein coupled receptor binding

Supervisor Prof. Michael Koelle (Dept. of Biophysics, Yale University, USA)

* Experimentally constructed libraries of *C.elegans* with desired genetic make-up
* Performed confocal imaging of *C.elegans* worms to find out neurons with neurotransmitter receptors
* Analyzed single-cell RNA sequencing data from the *C.elegans* gene expression map (CeNGEN) to confirm and cross check results obtained experimentally
* Actively participating on the research panel to improve the current CeNGEN project

**Post-Doctoral Research Associate** (2017 - 2019)

Title Activation of Erythropoietin Receptors by small artificial Transmembrane Proteins

Supervisor Prof. Daniel DiMaio (Department of Genetics, Yale University, USA)

* Used point mutational data generated in the lab to computationally engineer artificial transmembrane proteins (traptamers) that bind to human and mouse Erythropoietin Receptors (EPOR)
* Computational models for EPOR and traptamers interactions designed and tested using atomistic simulations to highlight the amino acid contacts necessary for binding and activation of EPORs
* EPOR activation by traptamers is driven by the subtle interplay of hydrophobic interactions mediated by surface-exposed residues of the receptor and traptamers
* Designed computational models currently guiding the design of novel experiments in the lab
* Investigated the role of traptamers in down-regulating the HIV co-receptor CCR5 resulting in the inhibition of HIV infection in human T-cells

**PhD thesis**

Title Sequence and Structural Determinants of Helices in Membrane Proteins

* Detailed and systematic analysis of helices in high resolution crystal structures of Helical Membrane Proteins reveals environment dependent position-specific sequence preferences at helix termini
* Mem brane environment and sequence preferences in turn dictate structural capping motifs in the helices
* An examination of 1134 TM helices enables the deconstruction of `helix kinks’ into 9 different types containing alternative helical conformations (*π* and 310 helices) that play a significant role in optimal helix packing and oligomerization of membrane proteins
* Molecular dynamics studies of modelled helices reveal that protonated Histidine side-chain anchors the helix in the membrane by formation of hydrogen bonds with phospholipid heads of the lipid bilayer

**Masters thesis**

Title Prediction of Galactose Binding sites in Proteins using Machine Learning Techniques: A Support Vector Machine based approach

* + - Curated and mined a high-resolution X-ray crystal structure dataset comprising of ligands such as Galactose, Mannose and Glucose
		- Trained Support Vector Machines using features such as amino acid composition in the ligand binding site, secondary structures of neighboring residues, solvent accessibility, backbone torsion angles as well as evolutionary information (PSI-BLAST matrix) and predict galactose binding sites
		- Prediction of Galactose binding sites achieved with 91% efficiency and a specificity of 83% when tested with protein structures of Mannose and Glucose

**Skills**

Programming Python, R, Perl/Bioperl, R/Bioconductor, sed, awk, Shell scripting, Matlab

Sequence Analysis BLAST-suite, ClustalW, MUSCLE, MUSTANG, Mummer, PIPmaker

NGS Data Analysis Quality control (fastqc, samtools); De novo and reference based assembly

(BWA-mem); Variant discovery and genotyping (vcfilter), RNA-seq (Cufflinks,

Tuxedo and Trinity pipelines, DESeq2, DEXSeq), ChIP-seq (MAC, DiffBind);

methylation data analysis (minfi); Galaxy pipelines

Machine learning WEKA, LIBSVM

Visualization tools Pymol, VMD, Rasmol, Jmol,

MD simulation tools AMBER, CPPTraj, GROMACS, NAMD

**Education**

2009 – 2016 **Ph.D., Bioinformatics and Computational Biology**, *Molecular Biophysics Unit, Indian Institute of Science*, India

2007 – 2009 **MSc in Bioinformatics**, *Savitribai Phule Pune University, Pune*, India

2004 – 2007 **BSc in Biotechnology**, *Savitribai Phule Pune University, Pune*, India

**Academic Peer-review Service**

**Peer- reviewed research articles for journals**

* EMBO journal – 1 article
* Plos Computational Biology – 1 article
* Frontiers in Bioinformatics – 3 articles
* Biochemistry and Biophysics Reports (2021) – 13 articles
* Journal of Biomolecular Structure and Dynamics (2021) – 10 articles

**Publications**

**Research Articles**

2022 Activated sputum eosinophils associated with exacerbations in children on mepolizumab Gabriella Wilson, James Knight, Qing Liu, *Ashish Shelar*, Emma Stewart, Xiaomei Wang, Xiting Yan, Joshua Sanders, Cindy Visness, Michelle Gill, Rebecca Gruchalla, Andrew H Liu, Meyer Kattan, Gurjit K Khurana Hershey, Alkis Togias, Patrice M Becker, Matthew Altman, William W Busse, Daniel J Jackson, Ruth R Montgomery, Geoffrey L. Chupp **Journal of Allergy and Clinical Immunology** (154,2, 2024)

2023 Subthreshold serotonin signals combined by G-proteins Gaq and Gas activate C.elegans egg laying muscles Andrew Olson, Allison Butt, Nakeirah Christie, *Ashish Shelar* and Michael Koelle **Journal of Neuroscience** , (43:21, 2023)

2022 Using NeuroPal Multicolor Fluorescence labeling to identify neurons in *C. elegans Ashish Shelar,* Emerson Santiago, Nakeirah Christie and Michael Koelle, ***Current Protocols*** (2:11, 2022)

2018 Regulation of CC chemokine receptor 5 (CCR5) stability by Lys-197 and by transmembrane protein aptamers that target it for lysosomal degradation, Petti, Lisa, Sara Marlatt, Yong Luo, Elizabeth Scheideman,*Ashish Shelar*, and Daniel DiMaio.  ***Journal of Biological Chemistry*: jbc-RA117**

2018 Analysis of Histidine side-chain interactions in model bilayers : An MD simulation approach, *Ashish Shelar* and Manju Bansal, ***Journal of Molecular Biology 5:2018***

2017 Single Methyl Groups can act as Toggle Switches to specify transmembrane Protein-Protein Interactions**,** He Li, Helena Steinocher, *Ashish Shelar*, Emily B. Cohen, Erin N. Heim, Birthe B. Kragelund, Gevorg Grigoryan, and Daniel DiMaio. ***Elife* 6:e27701**

2016 Helix Perturbations in Membrane Proteins Assist in Inter-helical Interactions and Optimal Helix Positioning in the Bilayer, *Ashish Shelar* and Manju Bansal, ***BBA Biomem, 1858(11):2804-2817***

2016 Data on Helix Perturbations in Membrane Proteins Assist in Inter-helical

Interactions and Optimal Helix Positioning in the Bilayer, *Ashish Shelar* and

Manju Bansal, ***Data in Brief 2016 Dec; 9: 781–802***

2014 Sequence and Conformational preferences at termini of α-helices in Membrane Proteins: Role of the Helix environment, *Ashish Shelar* and Manju Bansal, ***Prot: Struct,Func and Bioinfo;, 82(12):3420-36***

**Book Chapters**

2024 Innate Immune Mechanisms Associated With Exacerbations on Mepolizumab G Wilson, Q Liu, S Gautam, J Knight, A Shelar, E Stewart, C Visness, J Sanders, M Gill, RS Gruchalla, AH Liu, M Kattan, G Khurana Hershey, A Togias, PM Becker, MC Altman, WW Busse, DJ Jackson, RR Montgomery, GL Chupp, ***TERMINATOR: CONTROL OF AIRWAY INFLAMMATION AND IMMUNE RESPONSE IN ASTHMA, ATS,2024***

2024 Spatial Genomic Approaches to Investigate HOX Genes in Mouse Brain Tissues, Ashish Shelar and Anasuya Dighe, ***HOX Genes : Methods and Protocols*** (Ed Bony DeKumar and Ashish Shelar) Yale University, CT , 2024, 235-246

2013 Defining α-helix geometry by Cαatom trace vs (φ-ψ) torsion angles: A comparative analysis, *Ashish Shelar \** , Prasun Kumar \* and Manju Bansal, ***Biomolecular Forms and Functions*** (Ed. M. Bansal and N. Srinivasan) IISc, Bangalore, 2013, 116-127 \* - Both authors contributed equally

Experimental Protein purification, cloning, plating techniques, PCR, gel electrophoresis,

biology HPLC

**Awards and Fellowships**

2016 **Department of Science and Technology, Govt. of India Fellowship** to carry out Post-doctoral Research

2016 **Department of Biotechnology, Govt. of India Fellowship** to carry out Post-doctoral Research

2015 **Best Poster Prize** for Helix distortions in Membrane Proteins: Role in Inter-helical interactions and Folding of the Membrane Protein at Waltham, Massachusetts, USA *Award during PhD*

2015 **Carl Storm International Diversity Fellowship** to Attend the Gordon Research Conference on Membrane Protein Folding at Waltham, Massachusetts, USA *Award during PhD*

2013 **Department of Biotechnology, Government of India, Travel Fellowship** to attend the Membrane Protein Folding meeting at Seoul, South Korea *Award during PhD*

2013 **Best Poster Prize** for Position-specific analysis of helix termini in *α*-helices in Membrane Proteins at the International Conference on Biomolecular Forms and Functions, Bangalore, India *Award during PhD*

2009 **Dept. of Biotechnology (DBT) research fellowship** for pursuing PhD by Government of India *Award during Masters*

2009 **Secured All India Rank (AIR) -26** at the Bioinformatics National Certification

Examination (BINC), India *Award during Masters*

2009 National level entrance exam for admission into Indian Institute of Science and secured research fellowship to pursue PhD *Award during Masters*

2008 **DBT-Student fellowship** by University of Pune, India for notable academic performance *Award during Masters*

**Poster presentations**

2024 ***Annual American Society of Nephrology Meeting,*** San Diego, USA

Poster Title Analysis of kidney biopsies from patients with glomerulonephritis using Imaging Mass Cytometry

2024 ***Annual American Society of Nephrology Meeting,*** San Diego, USA

Poster Title Using Imaging Mass Cytometry to define the cell identities in Human acute kidney injury and Chronic kidney disease

2024 ***Annual American Society of Nephrology Meeting,*** San Diego, USA

Poster Title Understanding pathophysiology of AIN through spatial characterization of cell-cell interactions using imaging mass cytometry in a human biopsy cohort

2021 ***23rd International C.elegans conference***, San Diego, USA

Poster Title Mapping G Protein Coupled Neurotransmitter Receptor Expression Patterns in *C. elegans*

2015 **Gordon Research Conference on ‘Membrane Protein Folding’**, *Waltham, MA, USA*

Poster Title Helix distortions in Membrane Proteins: Role in Inter-helical interactions and Folding of the Membrane Protein

2013 **Biophysical Society Thematic Meeting on ‘Membrane Protein Folding’**, *Seoul, South Korea*

Poster Title Sequence and Conformational preferences at helix termini in Membrane Proteins

2013 **International Conference on Biomolecular Forms and Functions**, *Bangalore, India*

Poster Title Position-specific analysis of helix termini in *α*-helices in Membrane Proteins

2012 **Lipid-Protein Interactions in the Membrane:Implications for Health and Disease**, *Hyderabad,India*

Poster Title Defining α-helix geometry by Cαatom trace vs (*φ-ψ*) torsion angles: A comparative analysis

2010 **International Conference on Recent Advances in Bioinformatics**, *Bhubaneswar, India*

Poster Title Machine Learning Approaches to predict Galactose Binding Sites in Proteins

**Oral Presentations**

2024 ***Annual American Society of Nephrology Meeting,*** San Diego, USA

Poster Title Understanding pathophysiology of AIN through spatial characterization of cell-cell interactions using imaging mass cytometry in a human biopsy cohort

2021 ***Annual Worm Meeting***, San Diego, USA

Poster Title Mapping G Protein Coupled Neurotransmitter Receptor Expression Patterns in *C. elegans*

2012 Sequence and Conformational preferences at helix termini in Membrane Proteins at **MBU In-house symposium held at IISc, Bangalore, India**

2016 Helix distortions in Membrane Proteins: Role in Inter-helical interactions and Folding of the Membrane Protein at **Annual Meeting of the Indian Biophysical Society**

**Teaching Experience**

2024 **Conducted workshops and hands-on-training sessions for analysis of spatial genomic data using Xenium** for members of Yale School of Medicine and Yale New Haven Health Hospital

2010 **Conducted lectures and a hands-on training workshop on the Use of Support Vector Machines and their applications in biological systems**, *at Kalinga Institute of Information Technology*, Orissa

**Languages**

English **Fluent** *Medium of education.GRE score: Verbal: 540/800, Quantitative:800/800; Analytical Writing : 4.5/6*

German **Beginner** *Beginners course at Max Mueller Bhavan, Pune, India*

**References**

**Dr. James Knight** Department of Genetics, Yale University, CT, USA

Email: j.knight@yale.edu

**Professor Michael Koelle** Molecular Biophysics and Biochemistry Yale University, CT, USA

Email : michael.koelle@yale.edu

**Professor Daniel DiMaio** Department of Genetics, Yale University, CT, USA

Email: daniel.dimaio@yale.edu

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