

Nitin Kumar Singh (Curriculum Vitae)

WEB	<i>Github:</i> singhnitink <i>G-Scholar:</i> Nitin Kumar Singh	<i>Linkedin:</i> nitin-kumar-singh-163179b4 <i>Portfolio:</i> https://singhnitink.github.io
RESEARCH INTERESTS	Molecular Simulations, Computational Chemistry/Biology, Drug Discovery, Drug Delivery, Machine Learning, Enzyme engineering.	
WORK EXPERIENCE	Michigan State University East Lansing, United States Postdoctoral Researcher. <ul style="list-style-type: none">• Research Topic: “Evaluating the interactions of proteins and small molecules with biological membrane systems.”• Advisor: Dr Josh Vermaas	2024 - Present
EDUCATION	Indian Institute of Technology Gandhinagar, India PhD, Chemical Engineering. <ul style="list-style-type: none">• Dissertation Topic: “Investigating the role of charged residues in protein structural dynamics and adsorption.”• Advisor: Dr Mithun Radhakrishna Visvesvaraya National Institute of Technology , Nagpur, India M. Tech., Chemical Engineering <ul style="list-style-type: none">• Dissertation Topic: “Molecular dynamics simulations of peptide nanotubes and their application in drug entrapment.”• Advisor: Dr Piyush P. Wanjari Dr. APJ Abdul Kalam Technical University , Lucknow, India B. Tech., Biotechnology <ul style="list-style-type: none">• Dissertation Topic: “Production of Xylanase enzyme using agro-industrial waste by solid substrate fermentation and its process optimization.”• Advisor: Dr Santosh Kumar Mishra	2019 - 2024 2017 - 2019 2013 - 2017
INTERNSHIPS AND INDUSTRIAL TRAINING	<ul style="list-style-type: none">• Visiting Graduate Student: Understanding the interplay of helical stability and membrane interactions of charged peptides. Dr. Paulo C. T. Souza, École Normale Supérieure de Lyon and CNRS (August 2023- December 2023)• Summer Internship : Hindustan Coca-Cola Beverages Private Limited, Varanasi, Uttar Pradesh, India. (July-2016)• Summer Internship : Cytogene Research and Development, Lucknow, Uttar Pradesh, India. (June-2015)• Molecular Simulation and Computational Chemistry Software Packages: GROMACS, AMBER, NAMD, LAMMPS, Gaussian, GAMESS, Packmol, AutoDock Vina, Open Babel, HADDOCK.• AI-Based Structural Biology Tools: AlphaFold, RosettaFold.• High-Performance Computing: Experience in using Linux-based clusters (SLURM and PBS).	
TECHNICAL SKILLS		

TEACHING	<ul style="list-style-type: none"> • Programming Skills: Bash scripting, Batch scripting, Python, FORTRAN, Tcl scripting, HTML, PHP, MATLAB, Scikit-learn, TensorFlow, RDKit. • Visualization and Plotting Softwares: VMD, UCSF Chimera, PYMOL, Avogadro, gnu-plot, Grace, Matplotlib, Microsoft Excel, Graphpad-prism, Originlab. • Biotechnology Lab Operations: Gel Electrophoresis, Polymerase Chain Reaction, Spectroscopy and Spectrophotometry, Cell Culture. • Independent Tutor: Molecular Simulations (Theory and Application): Sem II, 2023-2024, Indian Institute of Technology Gandhinagar.
CERTIFICATIONS	<ul style="list-style-type: none"> • Machine Learning Specialization (Stanford University & DeepLearning.AI Coursera) • Hands-on Introduction to Linux Commands and Shell Scripting (Coursera) • Introduction to Networking and Storage (Coursera) • Project Management Principles and Practices Specialization (University of California, Irvine) • Certification in Scientific Writing (Indian Institute of Technology Gandhinagar)
PUBLICATIONS	<ul style="list-style-type: none"> • Nitin Kumar Singh, Manish Agarwal, and Mithun Radhakrishna. “Statistical analysis of the unique characteristics of secondary structures in proteins” Computational Biology and Chemistry(2024):108237. • Nitin Kumar Singh, Pratyasha Bhardwaj, and Mithun Radhakrishna. “Hydrophobicity - A single parameter for accurate prediction of disordered regions in proteins” Journal of Chemical Information and Modeling,63,16(2023):5375–5383. • Nitin Kumar Singh, Kartik Pushpavanam, and Mithun Radhakrishna. “Tuning Electrostatic Interactions to Control Orientation of GFP Protein Adsorption on Silica Surface” ACS Appl. Bio Mater. 7.2 (2023): 596-608. • Nitin Kumar Singh, Manish Agarwal, and Mithun Radhakrishna. “Understanding the helical stability of charged peptides” Proteins: Structure, Function, and Bioinformatics 91.2 (2023): 268-276. • Kumar, Avishek, Nitin Kumar Singh, Deepshikha Ghosh, and Mithun Radhakrishna. “Understanding the role of hydrophobic patches in protein disaggregation.” Physical Chemistry Chemical Physics 23, no. 22 (2021): 12620-12629. • Medesety, Padmesh, Hrushikesh M. Gade, Nitin Kumar Singh, and Piyush P. Wanjari. “Highly selective carbon capture by novel graphene-carbon nanotube hybrids.” Molecular Simulation 47, no. 16 (2021): 1326-1334.
AWARDS AND RECOGNITION	<ul style="list-style-type: none"> • Graduate Aptitude Test in Engineering (GATE) 2017- All India Rank 730 • 2nd position: Logo Quiz, Gems Society, DBT, IMSEC
CO-CURRICULAR ACTIVITIES	<ul style="list-style-type: none"> • General Secretary- Gems Society, Department of Biotechnology, IMS Engineering College. (2014-2015) • Volunteer at Rotary Club Ghaziabad. (2015 and 2017) • Represented IMSEC at ‘Swedish Embassy Quiz’. (2015)