

Full List of Publications:

Journal Articles:

1. S. Bajpai, C. R. A. Abreu, N. N. Nair, M. E. Tuckerman, *Solute Tempered Adiabatic Free Energy Dynamics for Enhancing Conformational Space Sampling*, *J. Chem. Theory Comput.* **21**, 5928 (2025). (DOI: [10.1021/acs.jctc.5c00717](https://doi.org/10.1021/acs.jctc.5c00717))
2. S. Singh, G. Kaul, M. Shukla, A. Akhir, S. Tripathi, A. Gupta, R. Bormon, N. N. Nair, S. Chopra, and S. Verma *Linear Antimicrobial Peptide, Containing a Diindolyl Methane Unnatural Amino Acid, Potentiates Gentamicin Against Methicillin-Resistant Staphylococcus aureus*, *Drug Dev. Res.* **86**, e70070 (2025). (DOI: [10.1002/ddr.70070](https://doi.org/10.1002/ddr.70070))
3. G. Dhanda, H. Singh, A. Gupta, S. A. Mohid, K. Biswas, R. Mukherjee, S. Mukherjee, A. Bhunia, N. N. Nair, and J. Halder *Dual-Functional Antibiotic Adjuvant Displays Potency against Complicated Gram-Negative Bacterial Infections and Exhibits Immunomodulatory Properties*, *ACS Cent. Sci.* **11**, 279 (2025). (DOI: [10.1021/acscentsci.4c02060](https://doi.org/10.1021/acscentsci.4c02060))
4. R. Javed, A. B. Kapakayala, and N. N. Nair *Buckets Instead of Umbrellas for Enhanced Sampling and Free Energy Calculations*, *J. Chem. Theory Comput.* **20**, 8450 (2024). (DOI: [10.1021/acs.jctc.4c00776](https://doi.org/10.1021/acs.jctc.4c00776))
5. S. Sen, R. Ali, A. Onkar, S. Verma, Q. T. Ahmad, P. Bhadauriya, P. Sinha, N. N. Nair, S. Ganesh, and S. Verma *Synthesis of a highly thermostable insulin by phenylalanine conjugation at B29 Lysine*, *Commun Chem* **7**, (2024). (DOI: [10.1038/s42004-024-01241-z](https://doi.org/10.1038/s42004-024-01241-z).)
6. S. Verma and N. N. Nair *A Comprehensive Study of Factors Affecting the Prediction of the pKa Shift of Asp26 in Thioredoxin Protein*, *J. Phys. Chem. B* **128**, 7304 (2024). (DOI: [10.1021/acs.jpcb.4c01516](https://doi.org/10.1021/acs.jpcb.4c01516))
7. P. Sarkar P, W. Xu, M. Vázquez-Hernández, G. Dhanda, S. Tripathi, D. Basak, H. Xie, L. Schipp, P. Dietze, J. E. Bandow, N. N. Nair, J. Halder *Enhancing the antibacterial efficacy of vancomycin analogues: targeting metallo-β-lactamases and cell wall biosynthesis*, *Chem. Sci.* **15**, 16307 (2024). (DOI: [10.1039/d4sc03577a](https://doi.org/10.1039/d4sc03577a))

8. Vaishali Thakkur, Chandan Kumar Das, Shivani Verma, Suman Saha, Nisanth N. Nair
Methyl substituted β -lactam framework based antibiotics and β -lactamase inhibitors: Proof of concept by computations, bioRxiv (2024). ([DOI: 10.1101/2024.01.14.575563](https://doi.org/10.1101/2024.01.14.575563))
9. Ritama Kar, Sagarmoy Mandal, Vaishali Thakkur, Bernd Meyer, Nisanth N. Nair
Speeding-up Hybrid Functional-Based Ab Initio Molecular Dynamics Using Multiple Time-stepping and Resonance-Free Thermostat, J. Chem. Theory Comput. **19** 8351 (2023). ([DOI: 10.1039/d3cp00521f](https://doi.org/10.1039/d3cp00521f))
10. Chandan Kumar Das, Abhinav Gupta, Nisanth N. Nair
Probing the general base for DNA polymerization in telomerase: a molecular dynamics investigation, Phys Chem Chem Phys **25**, 14147 (2023). ([DOI: 10.1039/d3cp00521f](https://doi.org/10.1039/d3cp00521f))
11. Shubhendra Tripathi, Nisanth N. Nair
Temperature Accelerated Sliced Sampling to Probe Ligand Dissociation from Protein, J. Chem. Inf. Model **63**, 5182 (2023) (DOI: [10.1021/acs.jcim.3c00376](https://doi.org/10.1021/acs.jcim.3c00376))
12. Shitanshu Bajpai, Brian Petkov, Muchen Tong, Charles Abreu, Nisanth N. Nair, Mark Tuckerman
An interoperable implementation of collective-variable based enhanced sampling methods in extended phase space within the OpenMM package, J. Comput. Chem. **44**, 2166 (2023). (DOI: <https://doi.org/10.1002/jcc.27182> & [10.26434/chemrxiv-2023-wwxq2](https://doi.org/10.26434/chemrxiv-2023-wwxq2))
13. Shivani Verma; Nisanth N. Nair
Computational Study of pKa Shift of Aspartate Residue in Thioredoxin: Role of Conformational Sampling J. Chem. Sci., **135**, 75 (2023). ([arXiv:2211.13637v1](https://arxiv.org/abs/2211.13637v1))
14. Sagarmoy Mandal, Ritama Kar, Bernd Meyer, Nisanth N. Nair
Hybrid Functional and Plane Waves based Ab Initio Molecular Dynamics Study of the Aqueous Fe2+/Fe3+ Redox Reaction, ChemPhysChem, **24**, e202200617 (2023); DOI: [10.1002/cphc.202200617](https://doi.org/10.1002/cphc.202200617)
15. Rahul Verma; Nisanth N. Nair
Proton-Exchange Reaction in Acidic Zeolites: Mechanism and Free Energetics, J. Phys. Chem. C, **126**, 19169–19177 (2022); DOI: [10.1021/acs.jpcc.2c06146](https://doi.org/10.1021/acs.jpcc.2c06146).
16. Vaishali Thakkur, Chandan Kumar Das, Nisanth N. Nair
Inhibition Mechanism of Class D β -Lactamases by Avibactam, ACS Catal. **12**, 10338–10352 (2022); DOI: [10.1021/acscatal.2c02693](https://doi.org/10.1021/acscatal.2c02693).

17. Abhinav Gupta, Shivani Verma, Ramsha Javed, Suraj Sudhakar, Saurabh Srivastava, Nisanth N. Nair
Exploration of high dimensional free energy landscapes by a combination of temperature-accelerated sliced sampling and parallel biasing, J. Comput. Chem. **43**, 1186-1200 (2022); DOI: [10.1002/jcc.26882](https://doi.org/10.1002/jcc.26882).
18. Sagarmoy Mandal, Ritama Kar, Tobias Klöffel, Bernd Meyer, Nisanth N. Nair
Improving the scaling and performance of multiple time stepping-based molecular dynamics with hybrid density functionals, J. Comput. Chem. **43**, 588-597 (2022); (DOI: [10.1002/jcc.26816](https://doi.org/10.1002/jcc.26816)).
19. Anji Babu Kapakayala, Nisanth N. Nair
Boosting the Conformational Sampling by Combining Replica Exchange with Solute Tempering and Well-Sliced Metadynamics, J. Comput. Chem. **42**, 2233-2240 (2021); ([DOI:10.1002/jcc.26752](https://doi.org/10.1002/jcc.26752) & [arXiv:2108.13641](https://arxiv.org/abs/2108.13641)).
20. Asit Pal, Subhendu Pal, Shivani Verma, Motoyuki Shiga, Nisanth N. Nair
Mean Force Based Temperature Accelerated Sliced Sampling: Efficient Reconstruction of High Dimensional Free Energy Landscapes, J. Comput. Chem. **42**, 1996-2003 (2021); ([DOI: 10.1002/jcc.26727](https://doi.org/10.1002/jcc.26727))
21. S. Mandal, V. Thakkur, Nisanth N. Nair, *Achieving an Order of Magnitude Speedup in Hybrid-Functional- and Plane-Wave-Based Ab Initio Molecular Dynamics: Applications to Proton-Transfer Reactions in Enzymes and in Solution*, J. Chem. Theory Comput. **17**, 2244 (2021). ([DOI: 10.1021/acs.jctc.1c00009](https://doi.org/10.1021/acs.jctc.1c00009))
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23. C. K. Das, Nisanth N. Nair *Elucidating the Molecular Basis of Avibactam Mediated Inhibition of Class A β -Lactamases*, Chem. Eur. J. **26**, 9639-9651 (2020).
24. S. Mandal, Nisanth N. Nair, *Efficient computation of free energy surfaces of chemical reactions using ab initio molecular dynamics with hybrid functionals and plane waves* , J. Comput. Chem. **41**, 1790 (2020).
25. Irfan Qayoom, Rahul Verma, Prem Anand Murugan, Deepak Bushan Raina, Arun Kumar Teotia, Saravanan Matheshwaran, Nisanth N. Nair, Magnus Taegil, Lars Lidgren, Ashok Kumar, *A biphasic nanohydroxyapatite/calcium sulphate carrier containing Rifampicin and Isoniazid for local delivery gives sustained and effective antibiotic release and prevents biofilm formation* , Scientific Reports **10**, 14128, (2020).

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30. K. Soniya, S. Awasthi, Nisanth N. Nair, Amalendu Chandra, *Transimination Reaction at the Active Site of Aspartate Aminotransferase: A Proton Hopping Mechanism through Pyridoxal 5'-Phosphate* , *ACS Catal.* **9**, 6726-6283 (2019).
31. S. Awasthi, Nisanth N. Nair, *Exploring high-dimensional free energy landscapes of chemical reactions* , *Wiley Interdisciplinary Reviews: Comput. Mol. Sci.* **9**, e1398 (2019).
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33. S. Mandal, J. Debnath, B. Meyer, Nisanth N. Nair *Enhanced sampling and free energy calculations with hybrid functionals and plane waves for chemical reactions* *J. Chem. Phys.* **149**, 144113 (2018).
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35. Shalini Awasthi, Shalini Gupta, Ravi Tripathi and Nisanth N Nair *Mechanism and Kinetics of Aztreonam Hydrolysis Catalyzed by Class-C β -Lactamase: A Temperature-Accelerated Sliced Sampling Study* *J. Phys. Chem. B.* **122**, 4299-4308 (2018).
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38. A Kumar, V Sudarkodi, Priya V Parandekar, Nishant K Sinha, Om Prakash, Nisanth N Nair, Sumit Basu *Adhesion between a rutile surface and a polyimide: a coarse grained molecular dynamics study* *Model. Sim. Mat. Sci. Eng.* **26**, 035012 (2018).
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41. Kalpana Tomar, Satyendra Soni, Pratibha Bhadauriya, Rashmi Parihar, Subramaniam Ganesh, Nisanth N. Nair, Gurunath Ramanathan *Mercuric Ion Sensing by an Overlapping β -turn Containing Peptide* *Chemistry Select* **2**, 8072-8075 (2017).
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44. Shalini Awasthi and Nisanth N. Nair *Exploring high dimensional free energy landscapes: Temperature accelerated sliced sampling* ' *J. Chem. Phys.* **146**, 094108 (2017).
45. Chandan K Das and Nisanth N. Nair *Hydrolysis of Cephalexin and Meropenem by New Delhi Metallo β -Lactamase: Substrate Protonation Mechanism is Drug Dependent* *Phys. Chem. Chem. Phys.* **19**, 13111-13121 (2017).
46. N. Vithani, S. Batra, B. Prakash, Nisanth N. Nair *Elucidating the GTP Hydrolysis Mechanism in FeoB, a Hydrophobic Amino Acid Substituted GTPase* *ACS Catal. (Letter)* **7** 902-906 (2017).

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48. Sooraj Kunnikuruvan, Priya V. Parandekar, Om Prakash, Tom K. Tsotsis, and Nisanth N. Nair *Insights into the Mechanism and Kinetics of Thermo-Oxidative Degradation of HFPE High Performance Polymer* J. Phys. Chem. B. **120**, 4852-4860 (2016).
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51. Shalini Awasthi, Venkat Kapil and Nisanth N. Nair *Sampling Free Energy Surfaces as Slices by Combining Umbrella Sampling and Metadynamics* J. Comput. Chem. **37**, 1413-1424 (2016).
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66. Venkataramana Imandi, Sooraj K., and Nisanth N. Nair *Hydroxypalladation Precedes Rate Determining Step in the Wacker Oxidation of Ethene* *Chem. Eur. J.* **19**, 4724-4731 (2013). [Highlighted as Very Important Paper]
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Conference Papers:

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2. Sooraj K., Nisanth N. Nair *Mechanism of oxidative degradation of PMR-15*, 2012 SAMPE International Symposium and Exhibition - Emerging Opportunities: Materials and Process Solutions; Baltimore, MD; United States
3. J. H. Franke, Nisanth N. Nair, L. Chi, H. Fuchs *Constrained density functional theory of molecular dimers*, High Performance Computing in Science and Engineering

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