

PUBLICATIONS:

50. Diship Srivastava, Shreya Mukherjee, Muskan Begom and Niladri Patra. **Modulation of Gramicidin A's Structural and Dynamical Properties by Cholesterol in the Membrane.** Submitted.

49. Diship Srivastava and Niladri Patra. **Improving the Computational Efficiency of the Adaptive Biasing Force Sampling by Leveraging the Telescopic-Solvation Scheme.** [J. Chem. Theory Comput.](#) 2024, 20, 24, 10952–10960.

48. Kanchan Negi, Ashok Kumar, Gourav Chakraborty, Sudhansubala Sahoo, Niladri Patra, Sumanta Kumar Sahu, **Rationally Designed Porous Self-Assembled Nanoparticles for Combinational ChemoPhotodynamic Therapy**, Dalton Trans. Dalton Trans., 2024,53, 17465-17479.

47. Sk. Akhter, Diship Srivastava, Aman Mishra, Niladri Patra, Pankaj Kumar, Sumanta Padhi, **A physicochemical investigation on Cu(II)-based molecular catalysts for the electrochemical reduction of CO₂ to syngas.** [Chem. Eur. J.](#) 2024, e202403321.

46. Abhishek Bera, Pritish Joshi, and Niladri Patra. **Delving into Macrolide Binding Affinities and Associated Structural Modulations in Erythromycin Esterase C: Insights into the Venus Flytrap Mechanism.** [J. Chem. Inf. Model.](#) 2024, 64, 15, 5964–5976.

45. Kousik Kumar Bhanja, Niladri Patra. **Discovery of Fourth-Generation Allosteric Inhibitors Targeting EGFR T790M/L858R/C797S and T790M/L858R Mutations: A Combined Machine Learning and Molecular Dynamics Approach.** submitted

44. Rakesh Kumar Roy, Madhur Sharma and Niladri Patra. **SARS-CoV-2 Spike Protein Variants and Bebtelovimab: Immune Escape Mechanisms Revealed by Computational Studies**, Phys. Chem. Chem. Phys., 2024,26, 29929-29939.

43. Gourav Chakraborty, Niladri Patra. **Targeting 14-3-3 ζ : α -Synuclein Complexation: Identification of Allosteric Sites and Development of Modulatory Inhibitors.** submitted

42. Gourav Chakraborty, Keka Ojha, Ajay Mandal, Niladri Patra, **Effect of spacer group variation of gemini surfactants on the detachment of oil from silica surfaces with different hydrophobicity: a molecular dynamics study**, Phys. Chem. Chem. Phys. Accepted

41. Kousik Kumar Bhanja, Madhur Sharma, Niladri Patra. **Computational Design of Allosteric Tyrosine Kinase Inhibitors Targeting Non-Small Cell Lung Cancer.** submitted.

40. Avigyan Naskar, Rakesh Roy, Niladri Patra. **Decoding Inhibitor Egression from Wild-Type and G2019S Mutant LRRK2 Kinase: Insights into Unbinding Mechanisms for Precision Drug Design in Parkinsons Disease**, J. Phys. Chem. B 2024, 128, 28, 6657–6669.

39. Gourav Chakraborty, Niladri Patra. **Elucidating the Molecular Basis of 14-3-3 Interaction with -Synuclein: Insights from Molecular Dynamics Simulations and the Design of a Novel Protein-Protein Interaction Inhibitor.** J. Phys. Chem. B 2024, 128, 29, 7068-7085.

38. Rakesh Roy, Abhishek Bera, Niladri Patra, **Insights into Allosteric Inhibition of AcrB Efflux Pump: Role of Distinct Binding Pockets, Protomer Preferences, and Crosstalk Disruption**, *J. Phys. Chem. B* 2024, 128, 29, 7068-7085.
37. Gourav Chakraborty, Mahima Sudhir Kolpe, Ambily Nath I.V, Avlokita Tiwari, Praapti Jayaswal, Niladri Patra, **Computational structure-guided approach to simulate delamanid and pretomanid binding to mycobacterial F420 redox cycling proteins: identification of key determinants of resistance**, *Journal of Biomolecular Structure & Dynamics*, accepted.
36. Debayan Basu, Barshali Ghosh, Diship Srivastava, Niladri Patra and Hari Pada Nayek, **Mononuclear Organogermanium(IV) Catalysts for [3+2] Cycloaddition Reaction**, *Dalton Trans.*, 2024,53, 5648-5657.
35. Abhishek Bera, Shreya Mukherjee, Niladri Patra. **Exploring the Transmembrane Allostery in MexB: DB08385 Variant as Promising Inhibitor like Candidate Against Pseudomonas aeruginosa Antibiotic Resistance – A Computational Study**, *Phys. Chem. Chem. Phys.*, 2024, 26, 17011-17027.
34. Diship Srivastava, Niladri Patra, **Elucidating Daptomycins Antibacterial Efficacy: Insights into the Tripartite Complex with Lipid II and Phospholipids in Bacterial Septum Membrane**, *J. Phys. Chem. B* 2024, 128, 18, 4414–4427.
33. Diship Srivastava, Biswajit Saha, Niladri Patra, **Design of Saccharide Based Organic Binder for Low-grade Iron Ore Pelletization using Atomistic Simulations and Machine Learning Methods**, *J. Mol. Graphics Modell.* 2024.
32. Abhishek Bera, Rakesh Roy, Pritish Joshi, Niladri Patra, **Machine Learning-Guided Discovery of AcrB and MexB Efflux Pump Inhibitors**, *J. Phys. Chem. B* 2024, 128, 3, 648–663.
31. Aman Mishra, Diship Srivastava, Niladri Patra, Sumanta Padhi, **Formate Dehydrogenase Activity by a Cu(II)-based Molecular Catalyst and Deciphering the Mechanism by DFT studies**, *Dalton Trans.*, 2024,53, 1209-1220.
30. Gourav Chakraborty, Ambily Nath I.V, Mukta Sharma, Jigar Sheth, Mahima Korib, Avlokita Tiwari, Niladri Patra, **In silico structural and mechanical insights into bedaquiline resistance associated with high-grade non-synonymous mutations in atpE, mmpR5, and pepQ**, *Journal of Biomolecular Structure & Dynamics*, 0, 1-13, 2023.
29. Avigyan Naskar, Kousik Kumar Bhanja, Rakesh Roy, Niladri Patra, **Structural insight into G2019S mutated LRRK2 kinase and brain- penetrant Type I inhibitor complex: A Molecular dynamics approach**. *Journal of Biomolecular Structure & Dynamics*, 1-21,2023.
28. Rakesh Roy, Niladri Patra, **Probing the pH Sensitivity of OprM: Insights into Metastable States and Semi-Open Conformation**, *J. Phys. Chem. B* 2024, 128, 3, 622–634.
27. Diship Srivastava, Niladri Patra, **Telescoping-Solvation-Box Protocol based Umbrella Sampling Method for Potential Mean Force Estimation**, *J. Chem. Inf. Model.* 2023, 63,

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26. Diship Srivastava, Niladri Patra, **Enhanced Uptake of Anticancer C6-Pep Dimer in Tumor Membrane Caused by Differential pKa in Acidic Tumor Microenvironment**, *J. Phys. Chem. B* 2023, 127, 45, 9747–9758.

25. Kousik Kumar Bhanja, Madhur Sharma, Niladri Patra, **Uncovering the structural and binding insights of dual inhibitors simultaneously targeting two distinct sites on EGFR kinase**, *J. Phys. Chem. B* 2023, 127, 50, 10749–10765.

24. Avigyan Naskar, Kousik Kumar Bhanja, Rakesh Roy, Niladri Patra, Role of the Residue Q1919 in Increasing Kinase Activity of G2019S LRRK2 Kinase: A Computational Study. *ChemPhysChem* 2023, e202300306.

23. Rakesh Roy, Abhishek Bera, and Niladri Patra. Encapsulation of testosterone and dihydrotestosterone into chiral carbon nanotubes: A molecular dynamics study. *J. Mol. Liq.* 376 (2023) 121426.

22. Diship Srivastava and Niladri Patra. Self-Uptake Mechanism of Polymyxin-Based Lipopeptide against Gram-Negative Bacterial Membrane: Role of the First Adsorbed Lipopeptide. *J. Phys. Chem. B* 2022, 126, 41, 8222–8232.

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18. Subhasis Dey, Soumya Chatterjee, Anjali Patel, Nirmalya Pradhan, Diship Srivastava, Niladri Patra, Arindam Bhattacharyya, Debasis Manna. Photoresponsive transformation from spherical to nanotubular assemblies: anticancer drug delivery using macrocyclic cationic gemini amphiphiles, *Chem. Comm.* 57 (38), 4646–4649.

17. Rakesh Roy, Niladri Patra, Configuration Flipping in Distal Pocket of Multidrug Transporter MexB Impacts the Efflux Inhibitory Mechanism, *ChemPhysChem*, 21 (23), 2516–2524.

16. Priyapratim Patra, Niladri Patra, Sagar Pal, Opposite swelling characteristics through changing the connectivity in a biopolymeric hydrogel based on glycogen and glycine, *Polym. Chem.* 11, 2630–2634 (2020).

15. Surajit Mondal, Niladri Patra, Hari Nayek, Sumit Hira, Soumit Chatterjee, Swapan Dey, Unusual absence of FRET in triazole bridged coumarin-hydroxyquinoline, an active sensor for Hg²⁺ detection, *Photochem. Photobiol. Sci.*, 2020, 19, 1211–1221.

14. Priyapratim Patra, Venkata Sundeep Seesala, Saundry Raj Soni, Rakesh Kumar Roy, Santanu Dhara, Animesh Ghosh, Niladri Patra, and Sagar Pal. Biopolymeric pH-Responsive Fluorescent Gel for in-vitro and in-vivo Colon Specific Delivery of Metronidazole and Ciprofloxacin; **Eur. Polym. J.** 114, 255 (2019).
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12. Niladri Patra and Alexie V. Tkachenko, Layer-by-layer Self-assembly of Patchy Particles as a Route to Complex Lattice Structure, **PRE** 96, 022601 (2017).
11. Niladri Patra, Efthymios I. Loannidis and Heather J. Kulik. Computational Investigation of the Interplay of Substrate Positioning and Reactivity in Catechol O-Methyltransferase. **PLOS ONE**, 11, 1 (2016).
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9. Irena Yzeiri, Niladri Patra, and Petr Král, Porous Carbon Nanotubes: Molecular Absorption, Transport, and Separation. **J. Chem. Phys.** 140, 104704 (2014).
8. Niladri Patra, Dominic A. Esan, and Petr Král, Dynamics of Ion Binding to Graphene Nanostructures, **J. Phys. Chem. C** 117, 10750 (2013), cover page.
7. Ryan M. Pearson, Niladri Patra, Hao-jui Hsu, Sayam Uddin, Petr Král, and Seungpyo Hong, Positively Charged Dendron Micelles Display Negligible Cellular Interactions. **ACS Macro Letters** 2, 77 (2013).
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