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Employment History

- Feb-2026 – Apr-2026 📌 **Assistant Professor**, SR University, Warangal, India.
- Jun-2025 – Sep-2025 📌 **Project Research Scientist**, Indian Institute of Technology, Bombay, India.
- Jun-2023 – Jun-2025 📌 **Postdoctoral Researcher**, Indian Institute of Technology, Bombay, India.

Academic Credentials

- Oct-2022 📌 **Doctor of Philosophy in Physics, Indian Institute of Technology (Indian School of Mines)**, Dhanbad, Jharkhand, India.
Thesis title: *Experimental and In Silico Studies of Biomolecular Interactions.*
- Jul-2016 📌 **Master of Science in Applied Physics and Ballistics, Fakir Mohan University**, Odisha, India. - 78.00%
- May-2014 📌 **Bachelor of Science in Physics, Utkal University**, Odisha, India. - 75.66%
- May-2011 📌 **12th Science, CHSE**, Odisha, India. - 65.50%
- July-2009 📌 **10th Secondary, BSE**, Odisha, India. - 85.50%

Research Interest

- Biomolecular interactions.
- Structural Bioinformatics.
- Computational Drug Discovery and Design.

Skills

- Languages 📌 Strong reading, writing, and speaking competencies for Odia, English, Hindi.
- Computational 📌 Homology modeling, Pharmacophore mapping, Molecular docking, Molecular dynamics, Computational quantum chemistry calculations, Cryo-EM single-particle analysis.
- Experimental 📌 Absorption spectroscopy, Steady-state and time-resolved fluorescence spectroscopy, Circular dichroism spectroscopy.
- Software and Coding 📌 MS Office, Statistical analysis using Origin, Python, GROMACS, Desmond, Gaussian 09, AutoDock Vina, VMD, PyMol, Chimera, RELION.
- Misc. 📌 Academic research, teaching, training.

Research Publications

Journal Articles (Equal Contribution: †)

- 1 **J. Rout**, S. Das, and S. Kaledhonkar, "In silico identification of potential inhibitors of mycobacterium tuberculosis dna gyrase from phytoconstituents of indian medicinal plants," *Computers in Biology and medicine*, vol. 199, p. 111 343, 2025, ISSN: 18790534.  DOI: <https://doi.org/10.1016/j.combiomed.2025.111343>
- 2 I. Pandiarajan, S. B. Walunj, N. Banerjee, **J. Rout**, S. Srivastava, S. Patankar, and S. Kaledhonkar, "Application of bio-layer interferometry for the analysis of ribosome-protein interactions," *Frontiers in Molecular Biosciences*, vol. 11, p. 1 398 964, 2024, ISSN: 2296-889X.  DOI: <https://doi.org/10.3389/fmolb.2024.1398964>
- 3 Nandeshwar, **J. Rout**, S. M. Panda, and U. Tripathy, "Phytoconstituents of ashwagandha as potential inhibitors of human islet amyloid polypeptide (hiapp): An in silico investigation," *Journal of Biomolecular Structure and Dynamics*, 2023.  DOI: [10.1080/07391102.2023.2259491](https://doi.org/10.1080/07391102.2023.2259491)
- 4 **J. Rout**, B. C. Swain, and U. Tripathy, "In silico investigation of spice molecules as potent inhibitor of sars-cov-2," *Journal of Biomolecular Structure and Dynamics*, vol. 40, no. 2, pp. 860–874, 2022, PMID: 32938313.  DOI: [10.1080/07391102.2020.1819879](https://doi.org/10.1080/07391102.2020.1819879)
- 5 B. C. Swain†, J. Rout†, and U. Tripathy, "Interaction of vitamin b12 with β -lactoglobulin: A computational study," *Journal of Biomolecular Structure and Dynamics*, vol. 40, no. 5, pp. 2146–2155, 2022, PMID: 33074063.  DOI: [10.1080/07391102.2020.1835731](https://doi.org/10.1080/07391102.2020.1835731)
- 6 **J. Rout**, B. C. Swain, S. Subadini, P. P. Mishra, H. Sahoo, and U. Tripathy, "Conformational dynamics of myoglobin in the presence of vitamin b12: A spectroscopic and in silico investigation," *International Journal of Biological Macromolecules*, vol. 192, pp. 564–573, 2021, ISSN: 0141-8130.  DOI: <https://doi.org/10.1016/j.ijbiomac.2021.10.030>
- 7 **J. Rout**, B. C. Swain, S. Subadini, P. P. Mishra, H. Sahoo, and U. Tripathy, "Spectroscopic and computational insight into the conformational dynamics of hemoglobin in the presence of vitamin b12," *International Journal of Biological Macromolecules*, vol. 189, pp. 306–315, 2021, ISSN: 0141-8130.  DOI: <https://doi.org/10.1016/j.ijbiomac.2021.08.096>
- 8 S. K. Verma, **J. Rout**, S. Biswas, and U. Tripathy, "Association of the types of alcoholic beverages and blood lipids: A community-based study," *Proceedings of the National Academy of Sciences, India Section B: Biological Sciences*, vol. 91, no. 1, pp. 73–80, 2021.  DOI: [10.1007/s40011-020-01192-0](https://doi.org/10.1007/s40011-020-01192-0)
- 9 **J. Rout**, B. C. Swain, P. P. Mishra, and U. Tripathy, "Spectroscopic insight into the interaction of dopamine with spherical gold nanoparticles," *Journal of Photochemistry and Photobiology B: Biology*, vol. 203, p. 111 770, 2020, ISSN: 1011-1344.  DOI: <https://doi.org/10.1016/j.jphotobiol.2019.111770>
- 10 **J. Rout**, B. C. Swain, Sakshi, S. Biswas, A. K. Das, and U. Tripathy, "A simulation study on the influence of energy migration and relative interaction strengths of homo- and hetero-fret on the net fret efficiency," *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 226, p. 117 599, 2020, ISSN: 1386-1425.  DOI: <https://doi.org/10.1016/j.saa.2019.117599>
- 11 B. C. Swain, S. K. Mukherjee†, J. Rout†, P. P. Mishra, M. Mukherjee, and U. Tripathy, "A spectroscopic and computational intervention of interaction of lysozyme with 6-mercaptopurine," *Analytical and bioanalytical chemistry*, vol. 412, no. 11, pp. 2565–2577, 2020.  DOI: [10.1007/s00216-020-02483-1](https://doi.org/10.1007/s00216-020-02483-1)

- 12 B. C. Swain, S. Subadini, **J. Rout**, Sakshi, P. P. Mishra, H. Sahoo, and U. Tripathy, "Biophysical study on complex formation between β -lactoglobulin and vitamin b12," *Food Chemistry*, vol. 312, p. 126064, 2020, ISSN: 0308-8146. DOI: <https://doi.org/10.1016/j.foodchem.2019.126064>
- 13 N. Chandra†, S. Biswas†, J. Rout†, G. Basu, and U. Tripathy, "Stability of β -turn in lar2c-n7 peptide for its translation-inhibitory activity against hepatitis c viral infection: A molecular dynamics study," *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, vol. 211, pp. 26–33, 2019, ISSN: 1386-1425. DOI: <https://doi.org/10.1016/j.saa.2018.11.056>

Conference Proceedings

- 1 **J. Rout** and U. Tripathy, "In silico investigation of sars-cov-2 spike protein inhibitor," in *Proceedings of the Sixteenth DAE-BRNS Biennial Trombay Symposium on Radiation and Photochemistry*, 2022, pp. 181–182.
- 2 **J. Rout**, B. C. Swain, S. Subadini, Sakshi, P. P. Mishra, H. Sahoo, and U. Tripathy, "Investigating the binding interaction between β -lactoglobulin and vitamin b12: A spectroscopic and computational approach," in *Biophysical Journal*, vol. 120, 2021, 205a.
- 3 **J. Rout**, B. C. Swain, and U. Tripathy, "Investigation of binding interaction of vitamin b12 with hemoglobin," in *Proceedings of the Fifteenth DAE-BRNS Biennial Trombay Symposium on Radiation and Photochemistry*, 2019, p. 184, ISBN: 978-81-940321-5-1.
- 4 **J. Rout**, B. C. Swain, P. P. Mishra, and U. Tripathy, "Interaction of dopamine with gold nanoparticles: A fluorescence spectroscopic investigation," in *Proceedings of PHOTONICS-2018*, 2018, TG1–C2, ISBN: 978-93-88653-41-1.

Books and Chapters

- 1 B. C. Swain, A. K. Das, **J. Rout**, S. Biswas, and U. Tripathy, "Fluorescence correlation spectroscopy: A highly sensitive tool for probing intracellular molecular dynamics and disease diagnosis," in *Optical Spectroscopic and Microscopic Techniques: Analysis of Biological Molecules*, H. Sahoo, Ed., Singapore: Springer Nature Singapore, 2022, pp. 177–195, ISBN: 978-981-16-4550-1. DOI: [10.1007/978-981-16-4550-1_8](https://doi.org/10.1007/978-981-16-4550-1_8)

References

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