KRISTU JAYANTI
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## Centre for Research & Development

### Research Supervisor (Guide) Profiles
### Discipline of Supervision: Forensic Science


**Dr. Shweta Singh**
Assistant Professor
Department of Forensic Science
School of Biological and Forensic Sciences


**Areas of Specialisation:**
Forensic Chemistry, Forensic Toxicology

Dr. Shweta Singh is a researcher with specialized expertise in molecular biophysics, computational toxicology, and biomolecular interactions. Her work primarily focuses on ligand–DNA and ligand–protein binding studies, employing integrated spectroscopic techniques alongside advanced computational approaches such as molecular docking and molecular dynamics simulations. Her research provides comprehensive insights into binding mechanisms, conformational dynamics, molecular stability, and energetics, while also addressing the toxicological implications of a wide range of compounds, including pharmaceuticals, pesticides, dyes, and natural products. In addition to her fundamental research contributions, she has demonstrated proficiency in analytical method development, particularly in QuEChERS-based LC-MS/MS techniques for the precise quantification of drugs in biological matrices. She has been awarded the prestigious Junior Research Fellowship (JRF) and Senior Research Fellowship (SRF) by the University Grants Commission (UGC). She has published several research articles in reputed international journals. Her work reflects a strong interdisciplinary approach, effectively bridging chemistry, biology, and toxicological and forensic sciences, with a balanced emphasis on both theoretical understanding and practical applications.

### Selected Publications:


**1.** Sharma, P., **Singh, S.**, Gopi, P., Rani, M. S. S., Singh, P., Pandya, P., & Ali, M. S. (2025). Evaluating the carcinogenic potential of trazodone hydrochloride via duplex DNA targeting: Molecular interaction, binding mechanism and affinity assessment via structural calculations. Journal of Pharmaceutical and Biomedical Analysis, 263. https://doi.org/10.1016/J.JPBA.2025.116881

**2**. Parvin, S. I., Mohammad, M., **Singh, S.**, Gopi, P., Khan, M. R., Parvej, H., Halder, U. C., Islam, M. M., Pandya, P., & Gazi, H. A. R. (2025). Structural basis of multi-target interactions of Henna Dye Lawsone: an experimental and theoretical evaluation. Journal of Biomolecular Structure and Dynamics. https://doi.org/10.1080/07391102.2025.2474060

**3**. **Singh**, P., Gopi, P., Rani, M. S. S., Sharma, P., Singh, S., Kaur, J., Ali, M. S., & Pandya, P. (2025). Biophysical and structural insights into Azamethiphos-DNA interactions. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 334. https://doi.org/10.1016/j.saa.2025.125934