Dr. FARHA ARSHI

Synthetic & Computational Chemist | DFT Modeling & Complex Synthesis

Anticancer Metallodrugs • Molecular Docking • Structure-Activity Relationships

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ResearchGate: researchgate.net/profile/Farha-Arshi | **Google Scholar:** scholar.google.com/citations?user=JAw7WC4AAAAJ

PROFESSIONAL SUMMARY

PhD researcher with 7 years of experience in inorganic and medicinal chemistry, specializing in the rational design and synthesis of ruthenium-based metallodrugs combined with computational studies (DFT, molecular docking, ADME). Designed and synthesized 10 novel Ru(III) and half-sandwich Ru-arene Schiff-base complexes as potential anticancer and antimycobacterial agents, and authored 5 peer-reviewed publications (24 citations, h-index 4). Seeking a postdoctoral position to advance computational drug discovery and the development of metal-based therapeutic candidates.

RESEARCH VISION & POSTDOCTORAL GOALS

Aiming to translate computational chemistry insights into viable metallodrug candidates through rational, structure-based design. Postdoctoral research interests include: in vivo behavior and pharmacokinetics of metal-based therapeutic agents; lead-compound optimization and structure-activity refinement; computational drug-discovery workflows for metal complexes; and the study of metallodrug-biomolecule interactions.

RESEARCH HIGHLIGHTS

- Designed and synthesized 10 novel Ru(III) and half-sandwich Ru-arene Schiff-base complexes as potential anticancer and antimycobacterial agents
- Applied DFT, molecular docking, HOMO-LUMO, and MEP analysis to investigate structure-activity relationships and predict biological behavior
- Authored 5 peer-reviewed publications (24 citations, h-index 4) and 1 preprint across reputable inorganic and medicinal chemistry journals
- Presented research at national and international conferences, including the 30th ISCB International Conference (ISBC-2025)
- Mentored junior researchers in synthesis, characterization, and computational workflows

WORK EXPERIENCE

Doctoral Researcher (Inorganic & Medicinal Chemistry)

University of Lucknow • Lucknow, India • 12/2020 - 01/2026 • Full-time

Conducted doctoral research on the design and development of ruthenium-based metal complexes as potential anticancer and antimycobacterial agents. Synthesized and characterized 10 novel Ru(III) and half-sandwich Ru-arene Schiff-base complexes using NMR, FT-IR, UV-Vis, single-crystal X-ray, and CHNS analysis. Applied computational techniques including DFT (GAUSSIAN), molecular docking, HOMO-LUMO, and MEP analysis to investigate structure-activity relationships. Biological evaluation (anticancer, antimycobacterial, and antioxidant) was carried out in collaboration with partner laboratories, with assay results interpreted alongside the computational findings to establish structure-activity relationships. Authored peer-reviewed publications, presented research at conferences, and mentored junior researchers in synthesis and computational workflows.

Trainee – Computational Approaches to Drug Design and Development (CADD)

CSIR – Central Drug Research Institute (CDRI) • Lucknow, India • 01/2019 - 03/2019 • Internship

Completed an intensive 8-week certificate program in computational drug design, including molecular modeling, virtual screening, molecular docking, and bioinformatics tools used in pharmaceutical research and drug discovery.

RESEARCH INTERESTS

Rational Drug Design • Structure-Based Drug Design • Computational Drug Discovery • Density Functional Theory (DFT) • Molecular Modeling • Molecular Docking • Structure-Activity Relationships • Coordination & Medicinal Chemistry • Anticancer Metallodrugs

Personal focus: bridging computational predictions with experimental validation to rationally design metal-based therapeutics for cancer treatment.

RESEARCH METRICS

Citations: 24	**H-index: 4**	**Publications: 5**
Preprints: 1	**Conference Papers: 1**	

EDUCATION

Ph.D., Chemistry
University of Lucknow • Lucknow, India • 12/2020 - 01/2026
Thesis Title: Synthesis, Characterization and Biological Evaluation of Ruthenium Complexes with Different Amines
Supervisor: Dr. Ashok Kumar Singh | University accredited with A++ Grade by NAAC

M.Sc., Chemistry
Isabella Thoburn Degree College • Lucknow, India • 07/2016 - 08/2018

B.Sc., Zoology, Botany, Chemistry
University of Lucknow • Lucknow, India • 06/2013 - 06/2016

PUBLICATIONS

Exploring Schiff Base and its Palladium Complexes: Synthesis, Characterization, Antimycobacterial Activity, DFT, Molecular Docking and ADME Studies • Journal of Molecular Structure • 01/2026
DOI: https://doi.org/10.1016/j.molstruc.2025.143704

New Ru(III) 2,6-Bis(2-Benzimidazolyl)Pyridine Complexes Bearing p-Sub-Benzyl Thiosemicarbazones Schiff Base: Synthesis, Characterization, DNA Binding and Anti-cancer Activity • Chemistry – An Asian Journal • 04/2025
DOI: 10.1002/asia.202500059

Design, Synthesis, and Biological Insights of Half Sandwich Ruthenium-Arene Schiff Base Complexes: Molecular Docking and DFT • ChemistrySelect • 01/2025
DOI: 10.1002/slct.202404895

Synthesis, DFT Calculation, DNA Binding, and Biological Evaluation of Some Mononuclear Ru(III) Complexes with 2,6-Bis(2-benzimidazolyl)pyridine Bearing Different p-Substituted Heterochalcones • Russian Journal of General Chemistry • 02/2023
DOI: 10.1134/S1070363223020202

Design, Synthesis, Theoretical, Spectroscopic and Molecular Docking Studies of Ruthenium and Zinc Complexes and their Antimycobacterial Study • Asian Journal of Chemistry • 11/2022
DOI: 10.14233/ajchem.2022.23867

Ampicillin-Derived Ruthenium Schiff Base Complexes as Emerging Anticancer and Antimicrobial Candidates: Synthesis, Characterization, DFT, ADME and Molecular Docking • Preprint
https://doi.org/10.2139/ssrn.5512074

CONFERENCES & PRESENTATIONS

Paper Presentation – Synthesis, Characterization, Molecular Docking and Biological Evaluation of Ruthenium Complexes
Aryabhat Institute of Academics and Research & Goel Institute of Higher Studies Mahavidyalaya (Affiliated to University of Lucknow)

Oral Presentation – Synthesis, Spectral Studies and Molecular Docking of Thiosemicarbazide Ligands and Ruthenium Complexes
National Seminar on Advancement and Strategies for Sustainable Development & Environmental Protection, Netaji Subhash Chandra Bose Govt. Girls P.G. College, Lucknow

Poster Presentation – 30th ISCB International Conference (ISBC-2025)
International Society for Chemical and Biological Sciences (ISCB)

Workshop: HPTLC – Technique and Applications (Virtual)
Anchrom Enterprises (I) Pvt. Ltd. & Smriti College of Pharmaceutical Education

TECHNICAL SKILLS

Core Areas: Coordination Chemistry | Medicinal Chemistry | Computational Chemistry

Computational Chemistry & Drug Design: DFT, HOMO-LUMO & MEP analysis (GAUSSIAN) | Molecular docking (AutoDock, Discovery Studio) | Computational / structure-based drug design (CADD) | ADME & drug-likeness prediction | QSAR | Python / RDKit | ChemDraw

Synthesis & Purification: Multistep inorganic & organometallic synthesis | Schiff-base ligand and Ru-complex synthesis | Column chromatography (silica / alumina)

Spectroscopy & Structural Characterization: 1H & 13C NMR | FT-IR | UV-Vis | Single-crystal X-ray diffraction | CHNS elemental analysis | Spectral data interpretation

Research & Professional: Scientific writing & peer-reviewed publication | Project management | Mentoring | Team collaboration