

Dr. Farha Arshi

Synthetic & Computational Chemist

ANTICANCER METALLODRUGS · MOLECULAR DOCKING · STRUCTURE-ACTIVITY RELATIONSHIPS

✉ farhaarshi02@gmail.com ☎ +91 70076 50527 🌐 drfarhaarshi.space ▶ Lucknow, India

🟢 ORCID 0000-0002-2891-5697 🔵 LinkedIn 🔵 ResearchGate 🔵 Google Scholar

10

RU COMPLEXES

5

PUBLICATIONS

1

PREPRINT

25

CITATIONS

4

H-INDEX

Rational Drug Design

Density Functional Theory (DFT)

Structure-Activity Relationships

Structure-Based Drug Design

Molecular Modelling

Coordination & Medicinal Chemistry

Computational Drug Discovery

Molecular Docking

Anticancer Metallodrugs



experimental results feed back to sharpen the next round of predictions

PROFILE

Inorganic and medicinal chemist specialising in ruthenium-based metallodrugs, uniting hands-on organometallic synthesis with computational design (DFT, molecular docking, ADME). Seeking a postdoctoral role applying structure-based computational design to advance metal-based therapeutic candidates from prediction toward validated leads.

EXPERIENCE

► Doctoral Researcher — Inorganic & Medicinal Chemistry

University of Lucknow, India · Dec 2020 – Jan 2026

- Built a structurally diverse library of ten ruthenium(III) and half-sandwich ruthenium-arene Schiff-base complexes as anticancer and antimycobacterial candidates.
- Executed multistep organometallic synthesis and confirmed every structure by $^1\text{H}/^{13}\text{C}$ NMR, FT-IR, UV-Vis, single-crystal X-ray diffraction and CHNS elemental analysis.
- Applied DFT, HOMO-LUMO and molecular electrostatic potential (MEP) analysis alongside AutoDock molecular docking to establish predictive structure-activity relationships.
- Coordinated anticancer, antimycobacterial and antioxidant evaluation with partner laboratories, interpreting the biology against the computational predictions.
- Mentored junior researchers in synthesis, spectroscopic characterisation and computational workflows.

► Trainee — Computational Approaches to Drug Design (CADD)

CSIR – Central Drug Research Institute (CDRI), Lucknow · Jan – Mar 2019

- Completed an intensive 8-week certificate programme in molecular modelling, virtual screening, molecular docking and bioinformatics tools applied to pharmaceutical drug discovery.

PUBLICATIONS

Five peer-reviewed papers and one preprint · 25 citations · h-index 4

1. Exploring Schiff Base and its Palladium Complexes: Synthesis, Characterization, Antimycobacterial Activity, DFT, Molecular Docking and ADME Studies. *Journal of Molecular Structure* (2026). [DOI](#)
2. 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* (2025). [DOI](#)
3. Design, Synthesis, and Biological Insights of Half-Sandwich Ruthenium-Arene Schiff Base Complexes: Molecular Docking and DFT. *ChemistrySelect* (2025). [DOI](#)
4. Synthesis, DFT Calculation, DNA Binding and Biological Evaluation of Mononuclear Ru(III) Complexes with 2,6-Bis(2-benzimidazolyl)pyridine Bearing p-Substituted Heterochalcones. *Russian Journal of General Chemistry* (2023). [DOI](#)
5. Design, Synthesis, Theoretical, Spectroscopic and Molecular Docking Studies of Ruthenium and Zinc Complexes and their Antimycobacterial Study. *Asian Journal of Chemistry* (2022). [DOI](#)
6. Ampicillin-Derived Ruthenium Schiff Base Complexes as Emerging Anticancer and Antimicrobial Candidates: Synthesis, Characterization, DFT, ADME and Molecular Docking. *SSRN (preprint)* (2024). [DOI](#)

EDUCATION

Ph.D., Chemistry

University of Lucknow · NAAC A++

Dec 2020 – Jan 2026

Thesis: Synthesis, Characterization and Biological Evaluation of Ruthenium Complexes with Different Amines · Supervisor: Dr. Ashok Kumar Singh

M.Sc., Chemistry

Isabella Thoburn Degree College, Lucknow

Jul 2016 – Aug 2018

B.Sc. (Zoology, Botany, Chemistry)

University of Lucknow

Jun 2013 – Jun 2016

Certificate — CADD

CSIR – Central Drug Research Institute

2019

TECHNICAL SKILLS

► Computational & Drug Design

DFT, HOMO-LUMO & MEP (GAUSSIAN) · Docking (AutoDock, Discovery Studio) · Structure-based design (CADD) · ADME & drug-likeness · QSAR · Python / RDKit · ChemDraw

► Synthesis & Purification

Multistep inorganic & organometallic synthesis · Schiff-base ligand and Ru-complex synthesis · Column chromatography

► Spectroscopy & Characterisation

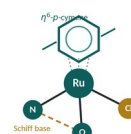
^1H & ^{13}C NMR · FT-IR · UV-Vis · Single-crystal X-ray diffraction · CHNS elemental analysis

► Research & Professional

Scientific writing & publication · Project management · Mentoring · Team collaboration

CONFERENCES

- **Poster** — 30th ISCB International Conference (ISCB-2025), International Society for Chemical and Biological Sciences.
- **Oral** — Thiosemicarbazide ligands and ruthenium complexes — National Seminar, Lucknow.
- **Paper** — Ruthenium complexes: synthesis, docking and biological evaluation — University of Lucknow.
- **Workshop** — HPTLC: Technique and Applications (Anchrom).



Half-sandwich Ru(II)-arene core — the scaffold of my doctoral work