ACADEMIC PROFILE

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AREA of INTEREST

1. **Organometallic Chemistry:** Organotin–protein/DNA interaction; Organotin–drug interaction.
2. **Organic/Medicinal Chemistry:** Designing novel anti-Alzheimer/antimicrobial/ antitubercular/anticancer/antiviral agents using *in silico* drug designing approaches.
3. **Green Chemistry:** Designing safer and less hazardous chemical synthesis.
4. **Heritage Chemistry:** History of Chemistry in Ancient India.

RESEARCH WORK

Present Areas of Research: Organotin Chemistry / Molecular Modeling / Computer Aided Drug Designing

Objectives:

- Design and synthesis of **organotin(IV) complexes with active drugs** with broad pharmacological profile and wide range of biological activities.
- Design and synthesis of **organotin(IV) complexes with Schiff bases** with opto-electronic applications.
- **Electronic structure calculations** of organotin(IV) complexes.
- Search **new molecules from natural leads** using *in silico* approaches with potential anti-Alzheimer/antimicrobial/ antitubercular/anticancer/antiviral activity.

Present Work:

- **Organotin(IV) complexes** of Drugs and/or Schiff bases containing heterocyclic systems (N/S/O donor atoms):
  Design, synthesis, and spectroscopic characterization (IR, NMR and Mass);
  Electronic structure calculations (**Density Functional Theory (DFT)-based computational studies**),
  Biological activity (Antimicrobial and anticancer/antitumour activity),
  Opto-electronic characterization (NLO and OLED), and
  Structure-activity relationship (SAR) studies.
- **Computer Aided Drug Designing**:
  Natural leads,
  Quantum-chemical calculations,
  In silico molecular Docking, and
  Quantitative Structure-activity Relationship (QSAR) studies.

LIST OF PUBLICATIONS (IN REFERRED JOURNALS):

1. New triorganotin(IV) complexes of quinolone antibacterial drug sparfloxacin: Synthesis, structural characterization, DFT studies and biological activity.

Applied Organometallic Chemistry, e3661 (**2018**). (doi: 10.1002/aoc.3661).
Corresponding author.

2. Combined experimental and theoretical studies on the diorganotin(IV) complexes of sparfloxacin: Synthesis, spectroscopic and DFT studies, and biological activity
   Journal of Molecular Structure, 1167, 44-56 (**2018**).
   ISBN: 0022-2860. Corresponding author.

3. Synthesis, spectroscopic characterization, biological activity and theoretical studies of E-N3-(2-chlorobenzylidene)-H-1,2,4-triazole-3,5-diamine.
   Journal of Molecular Structure, 1144, 324-337 (**2017**).
   ISBN: 0022-2860. Corresponding author.

4. An atoms-in-molecules (AIM) interpretation of organotin-peptide system: I. Di-*n*-butyltin(IV) derivative of glycyltryptophane.
   Asian Journal of Research in Chemistry, 10(2), 115-118 (**2016**).
   ISBN: 0974-4169 (Print); 0974-4150 (online). Corresponding author.

5. A density functional theory insight into the structure and reactivity of diphenyltin(IV) derivative of glycylphenyalanine.
   Main Group Metal Chemistry, 39 (3-4), 77-86 (**2016**).
   ISBN: 0792-1241 (Print); 2191-0219 (Online). Corresponding author.

6. Conceptual-DFT insights on the structure and reactivity of di-*n*-butyltin(IV) derivative of chlordiazepoxide.
   Journal of Indian Chemical Society, 93, 1053-1065 (**2016**).
   ISBN: 0019-4522. Corresponding author.

7. Structure and reactivity of di-*n*-butyltin(IV) derivative of chlordiazepoxide based on electronic structure calculations.
   Indian Journal of Chemistry Section A, 55A (8), 938-949 (**2016**).
   ISBN: 0376-4710 (Print); 0975-0975 (Online). Corresponding author.

8. An atoms-in-molecules analysis of the structure of di-*n*-butyltin(IV) derivative of glycylphenylalanine
   Chemical Science Review and Letters, 5(20), 171-175 (**2016**).
   ISBN: 2278-6783. Corresponding author.

9. Electronic structure calculations on dimethyltin(IV) derivative of glycylphenylalanine.
   International Journal of Current Science and Technology, 4(2), 215-220 (**2016**).
   ISBN: 2320-8090. Corresponding author.

10. A Density Functional Theory (DFT) study on di-*n*-butyltin(IV) derivative of glycyltryptophane.
    Asian Journal of Research in Chemistry, 9(2), 53-61 (**2016**).
    ISBN: 0974-4169 (Print); 0974-4150 (online). Corresponding author.

11. Theoretical insights on organotin(IV)-protein interaction: Density Functional Theory (DFT) studies on di-*n*-butyltin(IV) derivative of glycylvaline.
    Asian Journal of Research in Chemistry, 8(1), 7-12 (**2015**).

ISBN: 0974-4169 (Print); 0974-4150 (online). Corresponding author.

12. A density functional theory (DFT) perspective on organotin(IV)-drug interaction: dimethyltin(IV) derivative of chlordiazepoxide.
    Research Journal of Chemical Sciences, 4(11), 56-61 (**2014**).
    ISBN: 2231-606X. Corrsponding author.

13. New triorganotin(IV) derivatives of dipeptides as models for metal-protein interactions: synthesis, structural characterization and biological studies.
    Spectrochimica Acta Part A, 63, 66-75 (**2006**).
    ISBN: 1386-1425. Co-author (Ph.D. work).

14. New organotin(IV) derivatives of dipeptides as anti-inflammatory-antimicrobial agents. *European Journal of Medicinal Chemistry*, 40(3), 289-298 (**2005**).
    ISBN: 0223-5234. Co-author (Ph.D. work).

15. Diorganotin(IV) derivatives of dipeptides containing at least one essential amino acid residue: synthesis, characteristic spectral data, cardiovascular, and anti-inflammatory activities.
    Synthesis Reactivity in Inorganic and Metal-Organic Chemistry, 34(10), 1689-1708 (**2004**).
    ISBN: 0094 -5714 (Print); 1532-2440 (Online). Co-author (Ph.D. work).

16. New trimethyltin(IV) derivatives of dipeptides: synthesis, characteristic spectral studies and biological activity.
    Applied Organometallic Chemistry, 18, 460-470 (**2004**).
    ISBN: 1099-0739. Co-author (Ph.D. work).

17. New organotin(IV) derivatives of dipeptides as models for metal-protein interactions: in vitro anti-tumour activity.
    Applied Organometallic Chemistry, 17(5), 305-314 (**2003**).
    ISBN: 1099-0739. Co-author (Ph.D. work).

18. Comparative study of structure-activity relationship of di-and tri-organotin(IV) derivatives of amino acid and peptides.
    Journal of Organometallic Chemistry, 669, 109-123 (**2003**).
    ISBN: 0022-328X. Co-author (Ph.D. work).

19. Organotin(IV) complexes of amino acids and peptides.
    Coordination Chemistry Reviews, 215, 99-149 (**2001**).
    ISBN: 0010-8545. Co-author (Ph.D. work).

LIST OF PAPERS (IN CONFERENCES):

1. Combined quantum-chemical and molecular docking studies on some antimycobacterials as Inha and ADK inhibitors. (**Poster presentation)**
   6th International Symposium on Current Trends in Drug Discovery & Research, at CSIR-CDRI, Lucknow, from 25th to 28th of February, **2016**.

2. DFT based exploration on coordination behaviour of organotin(IV) derivatives of chlordiazepoxide. (**Poster presentation)**

18th CRSI National Symposium in Chemistry, at Panjab University, Chandigarh, from 5th to 7th of February, **2016**.

3. New facile synthesis of chromone derived azolopyrimidine. (**Poster presentation)**
   18th CRSI National Symposium in Chemistry, at Panjab University, Chandigarh, from 5th to 7th of February, **2016**.

4. Synthesis, Structural Characterization and DFT studies on diorganotin(IV) complexes of ciprofloxacin. (**Poster presentation)**
   18th CRSI National Symposium in Chemistry, at Panjab University, Chandigarh, from 5th to 7th of February, **2016**.

5. Combined quantum-chemical and molecular docking studies on some acetylcholinesterase inhibitors. (**Poster presentation**)
   International Conference on Nascent Developments in Chemical Sciences: Opportunities for Academia-Industry Collaboration, at BITS, Pilani, from 16th to 18th of October, **2015**.

6. DFT based investigations on diorganotin(IV) derivatives of glycyltyrosine. (**Poster presentation**)
   International Conference on Nascent Developments in Chemical Sciences: Opportunities for Academia-Industry Collaboration, at BITS, Pilani, from 16th to 18th of October, **2015**.

7. A density functional theory perspective on organotin(IV)-drug interaction: dimethyltin(IV) derivative of acesulfame-k. (**Poster presentation**)
   17th CRSI National Symposium in Chemistry, at CSIR-National Chemical Laboratory, Pune, from 6th to 8th of February, **2015**.

8. Density Functional Theory based investigations on dimethyltin(IV) derivative of tyrosinylphenylalanine. (**Poster presentation**)
   51st Annual Convention of Chemists, at Kurukshetra University, Kurukshetra, from 9th to 12th December, **2014**.

9. QSAR study on fungal fluconazole derivatives as ergosterol biosynthesis inhibitors. (**Poster presentation**)
   51st Annual Convention of Chemists, at Kurukshetra University, Kurukshetra, from 9th to 12th December, **2014**.

10. DFT studies on Schiff bases derived from substituted 1,2,4-triazole. (**Poster presentation**)
    Workshop on Introduction to Gaussian: Theory and Practice, at New Delhi, from 6th to 10th of January, **2014**.

11. Electronic structure and fluorescence characteristic of 5-aminoquinoline in acetonitrile:water binary mixture. (**Poster presentation**)
    National Symposium on Organic Synthesis and Advanced Materials, at Banaras Hindu University, Varanasi, from 1st to 2nd of March, **2014**.

12. Novel 1,2,4-triazole derived azomethines: synthesis and theoretical studies, (**Poster presentation**)
    National Symposium on Organic Synthesis and Advanced Materials, at Banaras Hindu University, Varanasi, from 1st to 2nd of March, **2014**.

13. Synthesis, docking and DFT studies on substituted 1,2,4-triazole derived Schiff bases as ergosterol biosynthesis inhbitors. (**Poster presentation**)
    National Symposium on Organic Synthesis and Advanced Materials, at Banaras Hindu University, Varanasi, from 1st to 2nd of March, **2014**.

14. Extraction and determination of Cu(II) ions by using ligand having nitrogen and sulphur donor atoms. (**Poster presentation**)
    15th CRSI National Symposium in Chemistry, at Banaras Hindu University, Varanasi, from 1st to 3rd of February, **2013**.

15. Dibutyltin(IV) derivatives of dipeptides. Synthesis, spectroscopic characterization (IR, $^{1}H/^{13}C$ NMR and ^{119}Sn Mössbauer), thermal studies and *in vitro* biological activity. (**Poster presentation**)
    88th Indian Science Congress, at New Delhi, from 3rd to 7th of January, **2001**.

16. Diphenyltin(IV) derivatives of amino acid and peptides. (**Oral presentation**)
    37th Annual Convention of Chemists, at Gurukul Kangri University, Hardwar, from 15th to 18th of November, **2000**.

ACADEMIC QUALIFICATIONS

Examination	Name of the Board/ University	Year of passing	Percentage of Marks obtained	Div./ Grade	Subjects
High School/ Matric	C.B.S.E., New Delhi	1988	66 %	I	English, Hindi, Mathematics, Science, Social Science
Intermediate/+2	C.B.S.E., New Delhi	1990	62.8 %	I	English, Mathematics, Physics, Chemistry, Biology
Graduation	Kumaun University, Nainital	1993	64.5 %	I	Physics, Chemistry, Mathematics
Post-Graduation (M.Sc.)	Kumaun University, Nainital	1995	66.3 %	I	Chemistry (Organic)
Other examinations (M. Phil.)	University of Roorkee, Roorkee	1998	75.4 %	I (With Hons.)	Chemistry (Industrial Methods of Chemical Analysis)

RESEARCH DEGREE(S)

Degree	Title	Date of Award	University
M.Phil.	Extraction and Determination of Metal Ions with the Ligands Containing Sulphur and Nitrogen Donor Atoms.	25.11.1998	University of Roorkee, Roorkee (Uttarakhand)
Ph.D.	Studies on Novel Organotin(IV) Derivatives of Peptides.	21.09.2005	Indian Institute of Technology-Roorkee, Roorkee (Uttarakhand)

AWARDS

1. University medal for securing first rank in the M.Phil. Course of Industrial Methods of Chemical Analysis in 1998 (University of Roorkee, Roorkee).
2. 3rd rank in order of merit of M.Sc. (Chemistry) course in 1995 (Kumaun University, Nainital).

FELLOWSHIPS AWAILED

1. Junior Research Fellowship (JRF-NET) from Council of Scientific & Industrial Research (CSIR), New Delhi (India), from March, 2000 to February, 2002, at the Indian Institute of Technology (IIT), Roorkee (India).
2. Senior Research Fellowship (SRF-NET) from CSIR, New Delhi (India), from March 2002 to October, 2004, at the Indian Institute of Technology, Roorkee (India).
3. Two months Science Academies Summer Research Fellowship (Teachers) during June, 2014-August, 2014 at CSIR-IICT, Hyderabad.

TEACHING PROFILE

Designation	Department	Date	
		From	To
Lecturer	Chemistry Group, Faculty Division-III, Birla Institute of Technology and Science (BITS), Pilani (Rajasthan).	03.01.2005	17.12.2005
Lecturer/Assistant Professor	Chemistry Section, Mahila Mahavidyalaya, Banaras Hindu University (BHU), Varanasi.	26.12.2005	05.03.2011
Assistant Professor	Chemistry Section, Mahila Mahavidyalaya, Banaras Hindu University (BHU), Varanasi.	16.03.2012	26.09.2017
Associate Professor	Chemistry Section, Mahila Mahavidyalaya, Banaras Hindu University (BHU), Varanasi.	27.09.2017	Till date

COURSES TAUGHT

Graduation: Organic Chemistry

B.Sc. Sem I: Organic Chemistry-I [Hydrocarbons, Reaction Mechanism, Stereochemistry, Alcohols and Active methylene compounds,].

B.Sc. Sem III: Organic Chemistry-II (2013-2014) [Carbonyl compounds, Aromatic nitrogen compounds].

B.Sc. Sem IV: Organic Chemistry-III [Carbohydrates, Dyes and Colour and constitution].

B.Sc. Sem V: Organic Chemistry-IV (2005-2006 to 2012-2013) [Cycloalkanes, Photochemistry].

B.Sc. Sem VI: Organic Chemistry-V (Since 2005-2006) [Amino acids, Carbohydrates, Terpenoids, Heterocyclic compounds].

Graduation: Physical Chemistry

B.Sc. Sem. I: Physical chemistry (2005-2006) [Electrochemistry]

B.Sc. Sem V: Physical Chemistry (Since 2006-2007) [Solid state, Electrochemistry]

B.Sc. Sem VI: Physical Chemistry-IV (Since 2006-2007) [Molecular spectroscopy]

Practical classes (all branches): Sem I to Sem IV.

Practical classes (Organic Chemistry): Sem V.

Post Graduation: M.Sc. Bioinformatics

Basics of Chemoinformatics (2006-2007 to 2007-2008)

Lab exercises based on chemoinformatics (2013-14 to till date).