Curriculum vitae

Saikat Mandal (He/Him/His)

Research Associate
Molecular, Cellular, and Developmental Biology
University of Michigan
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Born: 30th April, 1994, Murshidabad, India
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Academic details

2023 **Ph.D.**, Chemistry
National Institute of Technology Durgapur, Durgapur, India
Thesis Title: Bioactivity and anticancer property of Pt(II) & Pd(II) complexes of different bidentate chelates: their DNA/BSA binding, molecular docking and theoretical aspects
Supervisor: Prof. Sankar Chandra Moi, PhD, FRSC

2017 **M.Sc.**, Chemistry
University of North Bengal, Siliguri, India
First Class with Distinction (Marks: 71.31%)

2015 **B.Sc.** (Honours in Chemistry)
Kandi Raj College, University of Kalyani, Kalyani, India
Marks: 59%

Achievements

- **'Swami Vivekananda Merit-Cum-Means Scholarship'**, (Government of West Bengal) during M.Sc. (2015-2017)
- Qualified **GATE 2018** & **GATE 2019**

Experience

Research Experience

April, 2025-Present **Research Associate**
Supervisor- Dr. Randy Stockbridge, University of Michigan, USA
Duties: *Structural and functional characterization of membrane transporters.*

2023-2025 **Research Associate**
Supervisor- Prof. Lee Kroos, Michigan State University, USA
Duties: *To conduct biochemical, genetic, and microscopic experiments on mechanisms of signaling and gene regulation in Bacillus subtilis.*

2020-2023 **Senior Research Fellow**
DST-BT, Govt. of W. B. funded project
Supervisor- Prof. Sankar Ch. Moi, NIT Durgapur, India
Project Title: *Synthesis and characterization of cis-platin based Pt/Pd(II) complexes: Their kinetics mechanism, DNA-binding and theoretical study*

2018-2020 **Junior Research Fellow**
DST-BT, Govt. of W. B. funded project
Supervisor- Prof. Sankar Ch. Moi, NIT Durgapur, India
Project Title: *Synthesis and characterization of cis-platin based Pt/Pd(II) complexes: Their kinetics mechanism, DNA-binding and theoretical study*

2018, May-October **Project Assistant**
NIT Sikkim, India
Project Title: *Asymmetric synthesis of Bio active Natural Product and related Compound using Carbohydrate as Chiral Template*

Teaching Experience

2018-2023 **Teaching Assistant**
Teaching and Laboratory Instruction for conducting B.Tech. and M.Sc. classes at NIT Durgapur

Skills / Expertise:

- PCR, DNA isolation and purification, Plasmid Design and Construction, Site Directed Mutagenesis, Bacterial cell culture, SDS-PAGE, Immunoblotting, Protein purification.
- Organic and Inorganic synthesis, Column chromatography, Kinetic investigation, DNA and BSA binding activity through UV and fluorescence, Gel electrophoresis
- DFT, IRC, NBO calculation by Gaussian 09 software, Molecular Docking analysis by Autodock 4
- Cell Culture, MTT assay, NBT assay, DCFDA assay

Instruments handled

- UV-Vis Spectrophotometer (Shimadzu, UV-1800)
- Fluorescence Spectrophotometer (Hitachi, F-2500)
- FT-IR Spectrophotometer (Thermo Scientific, Nicolet iS10)
- Auto-titrator/ Titro-processor (Metrohm, 888 titrando)
- CHNS Analyzer (Thermo Scientific, Flash 2000)
- pH-meter, Conductometer
- Bio-Rad iMark Microplate Reader
- Bio-Rad Imager Gel Doc™ EZ
- FPLC

National and International Conference

- Poster presented at three days International Conference on "**Recent Developments in Chemistry**" (**RDC-2021**) organized by NIT Durgapur during March 3-5, 2021.
- Poster presented at two days International Conference on "**Molecules to Materials (MTM – 2020)**" organized by Department of Applied Chemistry, Sardar Vallabhbhai National Institute of Technology (SVNIT), Surat, Gujarat during December 17-18, 2020.
- Poster presented at "**ChemSci2020: Leaders in the Field Symposium**" organized by IISER Kolkata during December 7-10, 2020.
- Poster presented at three days National Conference on "**Recent Developments in Chemistry**" (**RDC-2018**) organized by NIT Durgapur during December 17-18, 2018.

Workshop and Short-Term Course

- Participated in International Workshop on "**Supporting Chemistry Research with Modern DFT (Density Functional Theory): Software, Techniques and Applications**" organized by Department of Chemistry, Smt. S. S. Patel Nootan Science & Commerce College, Gujrat during 4th-16th February 2021.
- Participated in Short Term Course on "**Applications of Computers in Chemistry**" at IIT Kharagpur on 11-13th March 2020.

Publications

1. M. A. Orlando†, H. J.T. Pouillon†, **S. Mandal**†, L. Kroos, and B. J. Orlando; Substrate Engagement by the Intramembrane Metalloprotease SpoIVFB; ***Nat Commun***, 15 (2024)8276. https://doi.org/10.1038/s41467-024-52634-6 **(†equal contribution)**

2. **S. Mandal**†, A. Soriano†, E. Smith, C. Erpelding, J. Ruffner, B. J. Orlando, L. Kroos; C-terminal part of BofA interacts with transmembrane segment of SpoIVFA; **Journal of Bacteriology**, 207 (2025) e00186 https://journals.asm.org/doi/10.1128/jb.00186-25 **(†equal contribution)**

3. **S. Mandal†,** S. Kumar Tarai†, P. Patra, P. Nandi, S. Sing, B. Rajak, S. C. Moi*, Brief Research on the Biophysical Study and Anticancer Behavior of Pt(II) Complexes: Their DNA/BSA Binding, Molecular Docking, and Cytotoxic Property, ***Langmuir***. 38 (2022) 13613. https://doi.org/10.1021/acs.langmuir.2c02490 **(†equal contribution)**

4. **S. Mandal**, S. Chatterjee, S. K. Tarai, A. Pan, R. Bhaduri, C. Das, Sankar Ch Moi, Synthesis and structural characterization of picolinamide and thiol chelated Pt (II) complexes: Their kinetics & mechanism and theoretical approach, ***Inorganica Chimica Acta***, 569 (2023) 122119. https://doi.org/10.1016/j.ica.2024.122119

5. **S. Mandal**, A. Pan, R. Bhaduri, S.K. Tarai, B.S. Kapoor, S.C. Moi, Theoretical investigation on hydrolysis mechanism of cis-platin analogous Pt(II)/Pd(II) complex by DFT calculation and molecular docking approach for their interaction with DNA & HSA, ***J. Mol. Graph. Model.*** 117 (2022) 108314. https://doi.org/10.1016/j.jmgm.2022.108314

6. **S. Mandal**, S.K. Tarai, A. Pan, R. Bhaduri, P. Biswas, S.C. Moi, Cytotoxic effects of Pd(II) complexes on cancer and normal cells: Their DNA & BSA adduct formation and theoretical approaches, ***Bioorg. Chem***. 128 (2022) 106093. https://doi.org/10.1016/J.BIOORG.2022.106093

7. **S. Mandal**, V. P. Reddy B, I. Mitra, S. Mukherjee, S. K. Tarai, R. Bhaduri, A. Pan, J. C. Bose K, G. K. Ghosh, S. C. Moi; Anticancer activity and biomolecular interaction of Pt(II) complexes: Their synthesis, characterization and DFT study; ***Appl. Organomet. Chem***. 36 (2022) e6506. https://doi.org/10.1002/aoc.6506

8. S. Chatterjee, **S. Mandal**, C. Das, R. Bhaduri, A. Bagchi, A. Biswas, S.C. Moi: Anticancer Activity of Picolinamide and Sulfur Chelated Pt(II) Complexes Against Breast Cancer: In Vitro Interaction Studies Through Molecular Docking With Bio-Receptors; **Chem. Asian J.**, 21 (2026) e70593. https://doi.org/10.1002/asia.70593

9. S. K.Tarai, **S. Mandal**, Arup Tarai, Ipsita som, Angana Pan, Arka Bagchi; Bio-physical study on DNA & BSA binding activity of Cu(II) complex: synthesis, molecular docking, cytotoxic activity and theoretical approach; ***Appl. Organomet. Chem***., (2023), e7164. https://doi.org/10.1002/aoc.7164

10. S. K. Tarai, **S. Mandal**, R. Bhaduri, A. Pan, P. Biswas, Ashish Bhattacharjee, S. C.Moi*; Bioactivity, molecular docking and anticancer behavior of pyrrolidine based Pt(II) complexes: their kinetics, DNA and BSA binding study by spectroscopic methods; ***Spectrochim. Acta A Mol. Biomol. Spectrosc***. 287 (2023) 122059. https://doi.org/10.1016/j.saa.2022.122059

11. R. Bhaduri, **S. Mandal**, S. Kumar Tarai, A. Pan, S. Mukherjee, A. Bagchi, A. Biswas, S. Ch. Moi*, Cytotoxic activity of nitrogen, sulfur, and oxygen chelated Pt(II) complexes; their DNA/BSA binding by in vitro and in silico approaches, ***J. Mol. Liq.*** 360 (2022) 119529. https://doi.org/10.1016/j.molliq.2022.119529

12. S. K. Tarai, **S. Mandal**, R. Bhaduri, A, Pan, V. P. Reddy B., K. Misra, S. C. Moi*; Theoretical hydrolysis mechanism of anticancer Pt(II) and Pd(II) dichloro complexes with N, N bidentate chelator in aqueous medium and their molecular docking; ***Chem. Phys.*** 553 (2022) 111390. https://doi.org/10.1016/j.chemphys.2021.111390

13. S. K. Tarai, A. Tarai, **S. Mandal**, B. Nath, I. Som, R. Bhaduri, Arka Bagchi, S. Sarkar, A. Biswas and S. C. Moi*; Cytotoxic behavior and DNA/BSA binding activity of thiosemicarbazone based Ni(II) complex: bio-physical, molecular docking and DFT study; ***J. Mol. Liq.***, 383 (2023) 121921. https://doi.org/10.1016/j.molliq.2023.121921

14. B. Ghosh, N. Roy, **S. Mandal**, S. Ali, P. Bomzan, D. Roy, Md S. Haydar, V. K. Dakua, A. Upadhyay, D. Biswas, K. K. Paul, M. N. Roy; Host–Guest Encapsulation of RIBO with TSC4X: Synthesis, Characterization, and Its Application by Physicochemical and Computational Investigations; ***ACS Omega***; 8 (2023) 6778. https://doi.org/10.1021/acsomega.2c07396

15. A. Pan, R. Bhaduri, **S. Mandal**, S. K. Tarai, A. Bagchi, A. Biswas, S. C. Moi; Photophysical study on DNA & BSA binding and cytotoxic behaviour of piperidine-Pt (II) complexes: Their kinetics & mechanism and molecular docking; **J. Photochem. Photobiol. A.**; 441 (2023) 114740. https://doi.org/10.1016/j.jphotochem.2023.114740

16. A. Pan, S. K. Tarai, R. Bhaduri, **S. Mandal**, S. C. Moi; Pd (II) based anticancer drug candidates with 1, 2-Aminoethyl piperidine scaffold and sulfur donor ancillary: Their in vitro bio-activity, molecular docking and DFT study; ***J. Mol. Liq.*** 386 (2023) 122421. https://doi.org/10.1016/j.molliq.2023.122421

17. B. Ghosh, N. Roy, D. Roy, **S. Mandal**, M. Mondal, V. K. Dakua, A. Dutta, S. Sen, A. Kumar, R. Chakraborty, M. N. Roy; Exploring Inclusion Complex of an Antithyroid Drug (PTU) with α-Cyclodextrin for Innovative Applications by Physicochemical Approach Optimized by Molecular Docking; 380 (2023) 121708. https://doi.org/10.1016/j.molliq.2023.121708

18. S. K. Tarai, R. Bhaduri, S. Mukherjee, **S. Mandal**, V. Pera Reddy B, S. C. Moi*; Drug reservoir mechanism of Pt (II)-sulfur chelates based on pharmacokinetics of Pt (II) complex with thiols & thio-ethers: An experimental and theoretical approach; ***Inorganica Chim. Acta*** 517 (2020) 120202. https://doi.org/10.1016/j.ica.2020.120202

19. R. Bhaduri, A. Pan, S. K. Tarai, **S. Mandal**, A. Bagchi, A. Biswas, S. Ch. Moi*; *In vitro* anticancer activity of Pd(II) complexes with pyridine scaffold: Their bioactivity, role in cell cycle arrest, and computational study; ***J. Mol. Liq.*** 367 (2022) 120540. https://doi.org/10.1016/j.molliq.2022.120540

20. B. Ghosh, N. Roy, D. Roy, **S. Mandal**, S. Ali, P. Bomzan, K. Roy, M. N. Roy*, An extensive investigation on supramolecular assembly of a drug (MEP) with βCD for innovative applications, ***J. Mol. Liq.*** 344 (2021) 117977. https://doi.org/10.1016/j.molliq.2021.117977

21. S. K. Tarai, A. Pan, P. Biswas, R. Bhaduri, **S. Mandal**, A. Paul, S. Baitalik, A. Bhattacharjee, S. C. Moi, Anticancer Behavior of Pyrrolidine-Based Palladium (II) Complexes and Biophysical Approach on Their DNA, BSA Binding Activity, Molecular Docking, and DFT Study, ***Langmuir*** 39 (2023) 10947–10964. https://doi.org/10.1021/acs.langmuir.3c01186

22. S.K. Tarai, A. Pan, S. Das, R. Bhaduri, **S. Mandal**, S. Maitra, S.C. Moi*, Anticancer property and normal cell toxicity profile of pyrrolidine based Platinum (II) complexes: Their DNA, BSA interaction and molecular docking, ***Appl. Organomet. Chem.*** n/a (2022) e6859. https://doi.org/10.1002/aoc.6859S

23. S. Mahata, S. Mukherjee, I. Mitra, R. Bhaduri, K. Chandra, **S. Mandal**, W. Linert, S. C. Moi*; Influence of steric and electronic effect of carrier ligand on kinetics & mechanism of Pt(II) complexes with l-cysteine and its substituted derivatives: Their experimental and DFT-based theoretical study; ***Inorganica Chim. Acta*** 498 (2019) 119117. https://doi.org/10.1016/j.ica.2019.119117

24. A. Pan, S. K. Tarai, A. Bagchi, T. Roy, R. Bhaduri, **S. Mandal**, K. Singh, M. Das, A. Biswas, S. C. Moi; In vitro bio-physical interaction of Pd (II) complexes with DNA and BSA: Their molecular docking and anticancer property; ***J. Mol. Liq.*** 437 (2025) 128468. https://doi.org/10.1016/j.molliq.2025.128468

Mentoring Experience

Throughout my PhD at NIT Durgapur (2018-2023), I mentored and trained several master's students who have successfully advanced to PhD programs at prestigious institutes across India. Below are examples of students I have guided:

Priya Patra (Current Position: PhD student at IIT Guwahati, India), Payel Nandi (Current Position: PhD Student at IISER Pune, India), Rituparna Saha (Current Position: NIT Agartala, India)

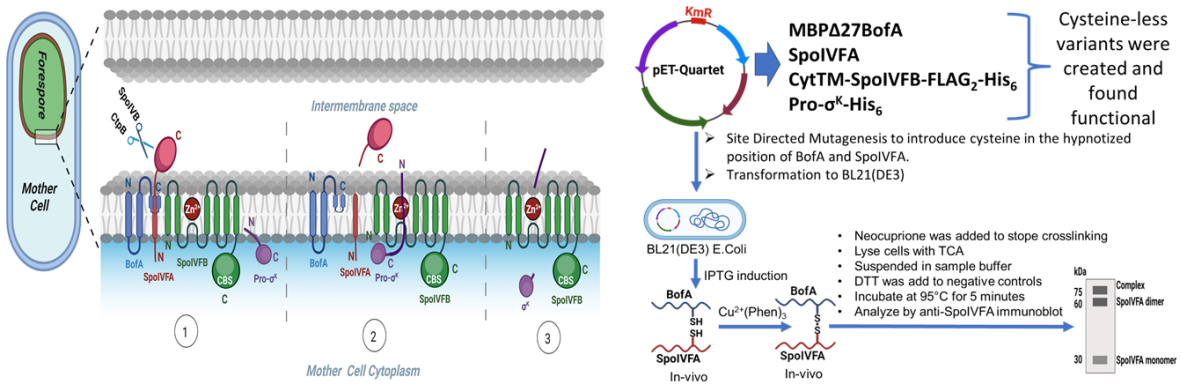
Peer review Experience

I have reviewed papers from following Journals.

Journals	Number of manuscripts reviewed
Langmuir (ACS)	1
ACS Omega (ACS)	3
Journal of Molecular Structure (Elsevier)	15
Journal of Molecular Graphics and Modelling (Elsevier)	1
Applied Organometallic Chemistry (Wiley)	1

Research Summary

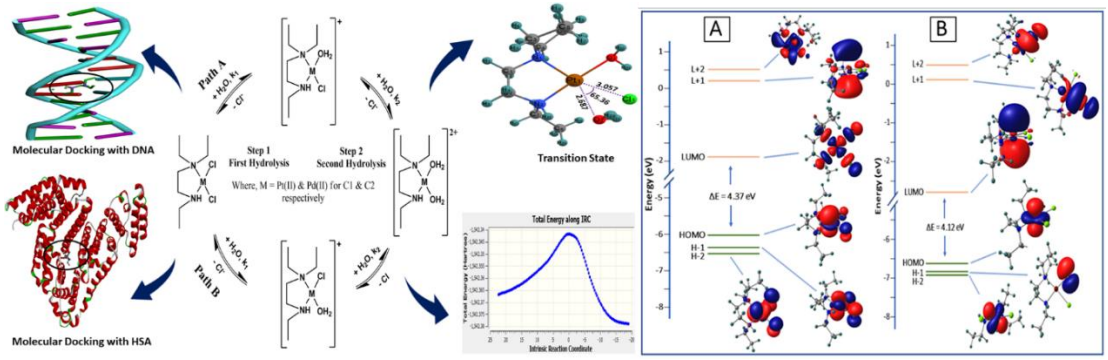
2023 – 2025, Michigan State University, USA



At MSU, I have worked on a research project on mechanisms of signaling and gene regulation in Bacillus subtilis. SpoIVFB is Intramembrane Metalloprotease that cleaves its substrate Pro-σ^K, allowing mature σ^K to diffuse from the outer forespore membrane into the mother cell cytoplasm and bind to RNA polymerase core subunits and initiate transcription of genes involved in the final stages of B. subtilis spore maturation. The homologs of SpoIVFB are very common in many bacteria for pathogenicity. Thus, understanding SpoIVFB could help to design better therapeutics. My project was focused on how Pro-σ^K engages with SpoIVFB in its active site and how SpoIVFB is inhibited by two inhibitory proteins BofA and SpoIVFA. I have performed various in vivo chemical crosslinking experiments between single cysteine mutants of these proteins to show how they interact with each other. [***Nat Commun***, 15 (2024)8276. https://doi.org/10.1038/s41467-024-52634-6]

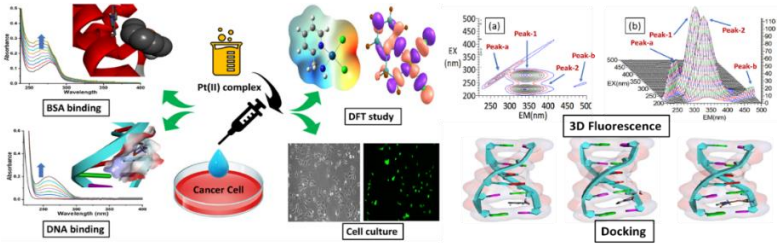
2018 – 2023, NIT Durgapur, India

1. Theoretical investigation of the kinetics and mechanism for the hydrolysis of cisplatin analogous complexes.



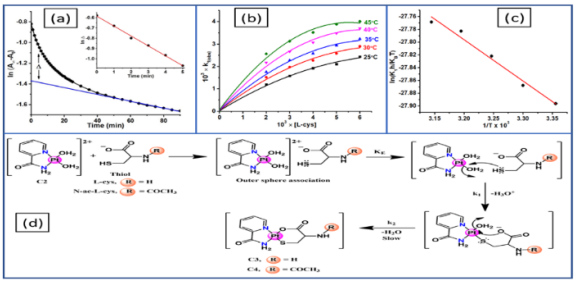
The mechanistic study on the hydrolysis of the Pt(II) dichloro complex is significant, which is concerned with the drug action before Pt(II)-DNA adduct formation as well as an understanding of DNA binding behaviour and, ultimately, the cell death mechanism. I have studied the hydrolysis mechanism of cisplatin analogous complexes using **DFT** calculation in different levels of theory. The transition states (TS) were identified and characterized by frequency calculation. **IRC** calculations were performed to confirm that the TS were well connected with reactants and products. HOMO-LUMO energy and MEP surface were calculated to determine the stability and reactivity of complexes. The activation energy of cisplatin analogous complexes was compared with recognized anticancer drugs. [***J. Mol. Graph. Model.*** 117 (2022) 108314. https://doi.org/10.1016/j.jmgm.2022.108314]

2. Synthesis of Pt(II)/Pd(II) complexes and their Biophysical Study and Anticancer Behavior: Their DNA/BSA Binding, Molecular Docking, and Cytotoxic Property



Researchers throughout the globe concentrate their research on finding a new and modified drug that has zero tolerance toxicity and minimum side effects. To achieve the goal, we modified Pt(II) based systems with different carrier ligands and labile groups. I have synthesized different series of Pt(II) as well as Pd(II) complexes, which are analogous to cisplatin. The interaction of these complexes with macromolecules (DNA and BSA) was investigated using UV-Vis spectroscopy, fluorescence spectroscopy, viscosity, cycle voltammetry, etc. The molecular docking technique was also applied for further analysis. The cytotoxicity of these complexes was evaluated on different cancer cell lines (A549, HCT116, MCF-7 etc) and normal cell lines (HEK293). The toxic effect in terms of ROS was evaluated using the DCFDA assay and NBT assay. Some of the complexes are found to have promising effects on cancer cells but very little effect on normal cells. [***Langmuir***. 38 (2022) 13613. https://doi.org/10.1021/acs.langmuir.2c02490]

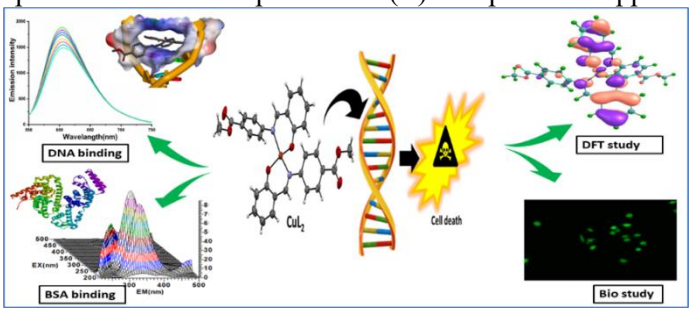
3. Kinetic investigation



Kinetics investigation is crucial and mandatory because anticancer complexes have to face the interaction with proteins and peptides, particularly thiols and thio-ether. Thus, kinetic study of Pt(II) complex with L-cysteine and N-acetyl-L-cysteine are considered as model reaction systems to evaluate their bind nature, binding constants and other thermodynamical parameters to propose and find out a mechanistic pathway. [***Appl. Organomet. Chem***., (2023), e7164. https://doi.org/10.1002/aoc.7164]

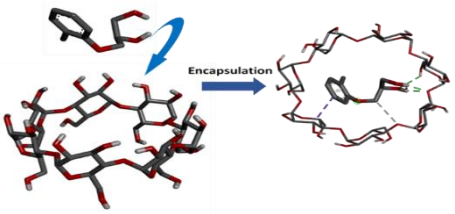
4. Synthesis of bioactive Schiff base and their metal (Cu) complex: their biophysical study for anticancer property.

We have tried to develop other transition metal chelated complexes that are cheaper than Pt(II) complexes. Copper complexes are regarded as suitable alternatives to platinum drugs among many bio-essential metals. In this context, Schiff bases are important due to their application in catalysis, anti-oxidative activity, and medicine such as antibiotics, anti-inflammatory agents, etc. We have synthesized Cu-Schiff base complexes and analyzed their potential application as anticancer drug candidates, which was verified by different biophysical studies. [***Appl. Organomet. Chem***., (2023), e7164. https://doi.org/10.1002/aoc.7164]



5. Encapsulation of drug molecules in β-Cyclodextrin nanocarrier: Innovative Physicochemical Applications

β-Cyclodextrin (β-CD) and p-sulfonatothiacalix[4]arene (TSC4X) are important container shape macrocyclic compound. They are hydrophilic in nature, whereas their internal cavities are relatively hydrophobic in nature. Thus, this type of molecule can act as a nanocarrier for polar and nonpolar small drug molecules by inclusion complex formation. The inclusion of complex formation can increase water solubility and minimize the doses in the human body. I have studied the inclusion complex formation of various drug molecule and their physiochemical application. [***J. Mol. Liq.*** 344 (2021) 117977. https://doi.org/10.1016/j.molliq.2021.117977]



2018, May-October, NIT Sikkim, India

1. Asymmetric synthesis of Bioactive Natural Product and related Compound using Carbohydrates as Chiral Template

References

Prof. Lee Kroos
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Department of Biochemistry and Molecular Biology
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Prof. Sankar Ch. Moi, Ph.D., FRSC
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