



Facultad de Medicina Universidad de Atacama Copiapó - Chile E-mail: haribabusiri970@gmail.com and jebiti.haribabu@uda.cl Phone no: +56982140027 (Chile) and +91-8792693593 (WhatsApp) https://scholar.google.co.in/citations?user=MLm_JEIAAAAJ&hl=en https://orcid.org/0000-0001-8855-032X https://www.scopus.com/authid/detail.uri?authorId=55621165400 https://www.webofscience.com/wos/author/record/ABH-8428-2020 https://publons.com/researcher/4117188/jebiti-haribabu/publications/ *Research website: https://sites.google.com/view/svsbmcl*



OBJECTIVE

Desiring a researcher position to carry out research/train young minds in the field of development of bioactive compounds for anticancer and antiviral applications.

CURRENT PROFILE

✓ Assistant Professor (06/03/2023 – Present) in Facultad de Medicina, Universidad de Atacama, Copiapó, Chile

ADDITIONAL RESPONSIBILITY

- ✓ Director (Alternate, 30/05/2023 Present) for Fondo de Innovación para la Competitividad (FIC) Projects (BIP code: 40049126-0, 40045256-0 and 40035624-0, (70000.00 USD)) in Facultad de Medicina, Universidad de Atacama, Copiapó, Chile
- ✓ Adjunct Faculty (21/06/2023 Present) in Chennai Institute of Technology, Chennai, India
- ✓ Special Yoga class (03/2023 Present) for Medical students in Facultad de Medicina, Universidad de Atacama, Copiapó, Chile

PROFESSIONAL EXPERIENCE

 National Fund for Scientific and Technological Development (FONDECYT) – Postdoctoral Research Fellow (17/11/2020 – 05/03/2023) in Universidad de Atacama, Copiapó, Chile
 Research: Design of Antitumoral Pt(II), Ru(II) and Ir(III) Complexes of Thiourea Ligands: Targeting Multiple mode of Action for Human Cancers (with Prof. Dr. E. Cesar)



- Japan Society for the Promotion of Science (JSPS) Postdoctoral Research Fellow (26/11/2018 15/11/2020) in Tokyo University of Science, Noda, Japan *Research:* Design and synthesis of green-emitting cationic peptide hybrids of cyclometalated Ir(III) complexes (IPHs) for biomedical applications (with **Prof. Dr. Shin Aoki**).
- Visiting Researcher (22/11/2017 25/03/2018) in Kaohsiung Medical University, Kaohsiung, Kaohsiung, Taiwan
 Research: Synthesis and characterization of Ru-arene complexes containing pyrazole based ligands for anticancer applications (with Dr. Sodio C. N. Hsu).
- Project Assistant (30/07/2012 01/04/2013) in CSIR-Central Leather Research Institute (CLRI), Chennai, Tamil Nadu, India *Research:* Technologies and products for solar energy utilization through networks (with Scientist Dr. T. Narasimhaswamy).

EDUCATION

UNIVERSIDAD **De Atacama**

- Doctor of Philosophy in Bioinorganic Chemistry (31/07/2013 28/07/2018, 90%) National Institute of Technology (NIT), Trichy, Tamil Nadu, India *Thesis Title:* DNA/protein binding and anticancer activity of Ni(II), Pd(II) and Ru(II) complexes bearing heterocyclic thiosemicarbazone ligands (Supervisor: Prof. R. Karvembu).
- Master of Science in Chemistry (6/2010 7/2012, 87.2%) Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India
 Project Title: Synthesis of novel spiroxyindoles for biological applications (with Dr. B.S.R. Reddy and Dr. N.C. Saradha).
- *Bachelor of Science in Chemistry and Biology* (6/2007 4/2010, 70.4%) Sri Venkateswara University, Tirupati, Andhra Pradesh, India

TEACHING EXPERIENCE

- ✓ I taught Chemistry and Biochemistry theory and practical classes for Medical Students at Facultad de Medicina, University of Atacama, Chile
- ✓ I taught Yoga classes for Medical Students at Facultad de Medicina, University of Atacama, Chile
- ✓ I taught theory and practical classes for national undergraduate (UG) and postgraduate (PG) students at NIT, Trichy, India.
- ✓ I taught practical classes for international undergraduate (UG) and postgraduate (PG) students at KMU, Taiwan.





RESEARCH INTERESTS

- Synthesis, characterization and biological applications of metal (Ni, Pd, Cu, Ir, Ru, Pt, Os, *etc.*) complexes with bioactive heterocyclic ligands
- Design, synthesis of luminescent cyclometalated Ir, Rh and Ru complexes containing cationic peptide hybrids for anticancer applications and bioimaging studies
- Synthesis, characterization and biomedical applications of heterocyclic compounds and bioactive organic compounds
- Delopment of organic and metal based biomarkers for medical applications
- Solution behaviour (aqueous chemistry), stability and biomolecules interactions (DNA, BSA, GSH, amino acids, *etc.*) of biologically active complexes UV-Vis, NMR, HPLC, mass spectrometry
- Anticancer and cell mechanistic studies of compounds (by MTT, Western blot, flow cytometry, confocal microscopy, cell cycle, *etc.*)
- Design, and synthesis of compounds for chemosensing applications for detecting toxic metals in real samples.
- Development of nanomaterials for biomedical applications

PRIZES AND AWARDS

- Stanford University publishes the World's Top 2% Scientists ranking and Clarivate Analytics publishes the Highly Cited Researchers list.
 This year's (2023) list is out and I am happy to be featured in the "Top 2% Scientists Worldwide" in the 2023 database, published by Stanford University, USA, and Elsevier BV.
- Selected for FONDECYT-Postdoctoral Research Fellow 2020 funding by Chile Government (Project No: 3200391) [Fellowship tenure: 11/2020 – 03/2023].
- Selected for prestigious Japan Society for the Promotion of Science (JSPS) 2018 funding by Japan Government (ID: P18412) [Fellowship tenure: 11/2018 – 11/2020].
- Selected for National Postdoctoral Fellowship (PDF/2018/001115) from Science and Engineering Research Board (SERB), Govt. of India, 2019.
- Young Scientist Award from Dr. K. V. Rao Scientific Society, Hyderabad, India, 2016-2017.
- Selected for Junior and Senior Research fellow awarded from University Grants Commission, Govt. of India, July 2013-July 2018.

NEWS AND MEDIA





I am listed in the "Top 2% Scientists Worldwide" in the 2023 database, published by Stanford University, USA, and Elsevier BV.

News Appared in "University of Atacama news letter and Redio" Link:<u>https://uda.cl/index.php?option=com_content&view=arti</u> cle&id=6370:cientifico-de-la-uda-que-desarrolla-farmacospara-tratar-el-cancer-destaca-entre-los-mejoresinvestigadores-del-mundo&catid=15:noticiasuda&Itemid=159

In News Paper "**El Diario de Atacama**" Link: https://www.diarioatacama.cl/impresa/2023/11/13/papel/

In Radio "Radio Marry"

Link: <u>https://www.maray.cl/cientifico-de-la-uda-destaca-</u> entre-investigadores-del-mundo-desarrolla-farmacos-contrael-cancer/

In news "Revista Minnera Crysol"

Link: <u>https://revistacrisol.cl/cientifico-de-la-universidad-de-atacama-destaca-entre-los-mejores-investigadores-del-mundo/</u>

In Radio "Radio Nostalgica"

Link: <u>https://www.nostalgica.cl/cientifico-de-la-uda-que-</u> desarrolla-farmacos-para-tratar-el-cancer-destaca-entre-losmejores-investigadores-del-mundo/ <image><text><text><text><text><text><text><text><text><text><text><text><text><text><text><text><text>









TV Interview about "My Research Highlights in TVn Atacama"



Link:

UNIVERSIDAD DE ATACAMA

> https://www.facebook.com/watch/?v=287007314328833 &ref=sharing



- My Invited talk on "How to Prevent Cancer Naturally?" at Govt. Degree College, Vedurukuppam, India, 27/09/2022, Appeared in Andhra Prabha local newspaper on 27 September 2022.
- My Invited talk on "Can a Health Lifestyles Avoid Cancer?" at Govt. Degree College, Nagari, Andhra Pradesh, appeared in Eenadu local newspaper on 20 September 2022.
- My Keynote talk in the International Webinar (NEC SH WEB TALKS-2K20) for Engineering and Science on "Role of Engineers in Drug Design: Molecular Docking Studies?" at National Engineering College, Kovilpatti, India, telecast on YouTube on 11th June 2020. Link: https://www.youtube.com/watch?v=NT0uYVRZuGw
- Japan Society for the Promotion of Science (JSPS) postdoctoral fellowship Award details were published in NIT, Trichy newsletter in August 2018.
- Young Scientist Award details were published in Dr. K. V. Rao Scientific Society winner book in 2017.

MEMBERSHIP

I have been a member of "Sociedad Farmacológica de Chile (SOFARCHI) or Pharmacological Society of Chile" in Chile since 2023.

REVIEWERS FOR INTERNATIONAL JOURNALS



క్యాన్సర్ అనువం నికిం కాదు నగరి: క్యాన్సర్ వ్యాధి అనువంశికం కాదని, జీవన విధానంలోని లోపం, ఆహా రష్మ అలవాట్ల లోపం కార ణంగా వస్తుందని (ప్రొఫెసర్ హారిబాబు పేర్కొన్నారు.











- ✓ Journal of Organometallic Chemistry (Elsevier Publications, from 2020)
- ✓ Polyhedron (Elsevier Publications, from 2021)

- ✓ Applied Organometallic Chemistry (Wiley Publications, from 2021)
- ✓ Advanced Materials Letter (International Association of Advanced Materials, from 2021)
- ✓ Inorganic Chemistry Communications (Elsevier Publications, from 2022)
- ✓ Journal of Biomaterials Science: Polymer Edition (Taylor and Francis Publications, from 2021)
- ✓ Results in Chemistry (Elsevier Publications, from 2022)
- ✓ International Journal of Polymeric Materials and Polymeric Biomaterials (Taylor and Francis Publications, from 2022)
- ✓ Heliyon (Elsevier Publications, from 2022)
- ✓ Process Biochemistry (Elsevier Publications, from 2022)
- ✓ Scientific Reports (Springer Nature Publications, from 2022)
- ✓ Molecules (MDPI Publications, from 2022)
- ✓ International Wound Journal (Wiley Publications, from 2022)
- ✓ ACS Omega (ACS Publications, from 2022)
- ✓ International Journal of Molecular Sciences (MDPI Publications, from 2022)
- ✓ Crystals (MDPI Publications, from 2022)
- ✓ Journal of Materials Research (Springer Nature Publications, from 2022)
- ✓ Journal of Nanoparticle Research (Springer Nature Publications, from 2022)
- ✓ Transition Metal Chemistry (Springer Nature Publications, from 2022)
- ✓ Int. J. of Bioinformatics Research and Applications (IJBRA) (Inderscience Submissions, from 2022)
- ✓ Biometals (Springer Nature Publications, from 2023)
- ✓ International Journal of Biological Macromolecules (Elsevier Publications, from 2023)
- ✓ Chemistry and Biodiversity (Wiley Publications, from 2023)
- ✓ Drug Research (Thieme Medical Publishers, from 2023)
- ✓ Current Topics in Medicinal Chemistry (Bentham Science Publishers, from 2023)
- ✓ Chemical Engineering Science (Elsevier Publications, from 2023)
- ✓ The Natural Products Journal (Bentham Science Publishers, from 2023)



- ✓ Marine Drugs (MDPI Publications, from 2023)
- ✓ BioChip Journal (Springer Nature Publications, from 2023)
- ✓ Journal of Drug Delivery Science and Technology (Elsevier Publications, from 2023)
- ✓ Chemical Papers (Springer Nature Publications, from 2023)
- ✓ ChemistrySelect (Springer Nature Publications, from 2024)
- ✓ Sensors (MDPI Publications, from 2024)
- ✓ Journal of Inorganic Biochemistry (Elsevier Publications, from 2024)
- ✓ Toxicology in Vitro (Elsevier Publications, from 2024)
- ✓ Journal of King Saud University Science (Elsevier Publications, from 2024)

PUBLICATION ACTIVITY (As per Google Scholar on 11-05-2024)

- **Total Publications: 106** published
 - ✓ **Full papers or communications: 87** published
 - ✓ **Review papers: 6** published
 - ✓ Structure Reports: 12 published
- ✤ Books: 1 published

UNIVERSIDAD DE ATACAMA

- Book Chapter: 1 published
- **Citations: 2510**
- ✤ H-index : 30 and i10-index: 60

LIST OF PUBLICATIONS (COMMUNICATIONS / FULL PAPERS / REVIEW ARTICLES)

- Michael addition-driven synthesis of cytotoxic palladium(II) complexes from chromone thiosemicarbazones: Investigation of anticancer activity through *in vitro* and *in vivo* studies <u>J. Haribabu</u>,* N. Balakrishnan, S. Swaminathan, D.P. Dorairaj, M. Azam, M.K. Mohamed Subarkhan, Y.-L. Chang, S.C.N. Hsu, P. Štarha, R. Karvembu, *New J. Chem.*, 2023, 47, 15748-15759, (Impact factor (IF): 3.98, Corresponding Author).
- 2. Effect of coordination mode of thiosemicarbazone on the biological activities of its Ru(II)benzene complexes: Biomolecular interactions and anticancer activity via ROS-mediated mitochondrial apoptosis

*J. Haribabu**, R. Arulkumar, D. Mahendiran, K. Jeyalakshmi, S. Srividya, P. Venuvanalingam, N. Bhuvanesh, J.F. Santibanez, R. Karvembu, *Inorganica Chim. Acta*, 2024, 565, 121973 (IF: 2.98, Corresponding Author).





Bis(acylthiourea) compounds as enzyme inhibitors: Synthesis, Characterization, Crystal structures and *in silico* molecular docking studies
 P. Jerome, *J. Haribabu*, * D.P. Dorairaj, M. Azam, G. Madhavan, D. Gayathri, R. R-Tagle, N. Bhuvanesh, M.J. Gallardo-Nelson, T.H. Oh, *J. Mol. Struct.*, 2024, 1297, 136977, (IF: 3.81, Corresponding Author).

UNIVERSIDAD DE ATACAMA

- Hinged bipodal furoylthiourea-based Ru(II)-arene complexes: Effect of (ortho, meta, or para)substitution on coordination and anticancer activity
 S. Swaminathan, *J. Haribabu*, D. Mahendiran, N. Maroli, J.J. Prakasan, N. Balakrishnan, N. Bhuvanesh, C. Echeverria, R. Karvembu, *Inorg. Chem.*, 2023, 62, 3679-3691, (IF: 5.16).
- Ru(II)-*p*-cymene Complexes of Furoylthiourea Ligands for Anticancer Applications Against Breast Cancer Cells
 P. Dorairaja, *J. Haribabu*, M. Dharmasivam, R.E. Malekshahd, M.K.M.Subarkhane, C. Echeverria, R. Karvembu, *Inorg. Chem.*, 2023, 62, 30, 11761–11774, (IF: 5.16).
- Copper(I) Complexes of Acylthiourea Ligands: Structural Insights and Cytotoxic Potential P. Arockia Doss, M. Dharmasivam S. Srividya, *J. Haribabu*, C. Echeverria, N. Bhuvanesh, R. Karvembu, *Appl. Organomet. Chem.*, 2024, e7474 (IF: 4.07).
- Recent progress in designing heterogeneous COFs with the photocatalytic performance
 S. Gharanli, R. E. Malekshah, M. Moharramnejad, A. Ehsani, M. Shahi, A. H. Joshaghani, A. H. Amini, <u>J. Haribabu</u>, E. S. Istifli, F. K. Tehrani, *Molecular Catalysis*, 2024. 560, 114127 (IF: 4.60).
- An ESIPT active coumarin-diphenyl azine-based AIEgen: Nanomolar Cu2+ ion sensing, Latent Fingerprinting, live-cell imaging, and real sample analysis
 A. Jain, S. Dea, P. Saraswat, *J. Haribabu*, J. F. Santibanezd, P. Barman, *J. Mol. Struct.*, 2024, Accepted, DOI: 10.1016/j.molstruc.2024.138383 (IF: 3.81).
- Synthesis of nitrogen-doped graphene oxide by nanosecond pulsed laser ablation of graphene in liquid for bioimaging applications
 R. Puliyasseri, *J. Haribabu*, R. Ramirez-Tagle, D. Sastikumar, *Diam. Relat. Mater.*, 2024, 143, 110909, (IF: 4.10).
- Copper-mediated cyclization of thiosemicarbazones leads to 1,3,4-thiadiazoles: Structural elucidation, DFT calculations, in vitro biological evaluation and in silico evaluation studies V. Manakkadan, *J. Haribabu*, N.V. Palakkeezhillam, P. Rasin, R. Vediyappan, V.S. Kumar, N. Bhuvanesh, A. Sreekanth, *Spectrochim. Acta A*, 2024, 313, 124117 (IF: 4.80).
- 11. Host-guest interactions of coumarin-based 1,2-pyrazole using analytical and computational methods: Paper strip-based detection, live cell imaging, logic gates and keypad lock applications

P. Rasin, S.M. Basheer, <u>J. Haribabu</u>, K.N. Aneesrahman, V. Manakkadan, V.N.V. Palakkeezhillam, N. Bhuvanesh, E. Cesar, J.F. Santibanez, A. Sreekanth, *Heliyon*, 2024, 10, e24077 (IF: 4.00).

12. Unraveling the Anticancer Efficacy and Biomolecular Properties of Ru(II)-Arene Complexes of Pyrene-Based Thiosemicarbazone Ligands: A Comprehensive In-Silico/ In-Vitro Exploration





V.N.V. Palakkeezhillam, *J. Haribabu*, V.S. Kumar, M. Azam, V. Manakkadan, P. Rasin, N. Bhuvanesh, A. Sreekanth, *Organometallics*, 2024, 43, 242–260, (IF: 3.83).

- A review of recent developments of metal–organic frameworks as combined biomedical platforms over the past decade
 M. Moharramnejad, R.E. Malekshah, A. Ehsani, S. Gharanli, M. Shahi, S.A. Alvan, Z. Salariyeh, M.N.Azadani, *J. Haribabu*, Z.S. Basmenj, A. Khaleghian, H. Saremi, Z. Hassani, E. Momeni, *Adv. Colloid Interface Sci.*, 2023, 316, 102908, (IF: 15.19). Review article.
- Study of the reaction mechanism in hydrogen production using metal-free Schiff base as a catalyst
 J. P. Muena, P. P. Zamora, K. Bieger, A. Soliz, <u>J. Haribabu</u>, M.J. Aguirree, P. Márquez, D. Quezada, J. Honoresh, J. Mol. Liq., 2023, 391, 123207, (IF: 6.63).
- Influence of indole-*N*-substitution of thiosemicarbazone in the cationic Ru(II)-(η⁶-benzene) complexes on their anticancer
 N. Balakrishnan, <u>J. Haribabu</u>, D. Mahendiran, D. Anandakrishnan, S. Swaminathan, N. Bhuvanesh, C. Echeverria, R. Karvembu, *Organometallics*, 2023, 42, 259–275, (IF: 3.83).
- Cytotoxicity of Cu(I) complexes containing indole-based thiosemicarbazones and triphenylphosphine
 P. Arockia Doss, <u>J. Haribabu</u>, N. Balakrishnan, S. Srividya, N. Bhuvanesh, J. P. Reyes, R. Karvembu, *ChemistrySelect*, 2023, 8, e202301277, (IF: 3.41).
- Effective and Selective Ru(II)-Arene Complexes Containing 4,4'-Substituted 2,2' Bipyridine Ligands Targeting Human Urinary Bladder Cancer Cells M. Murali, J.R. Chen, J. Haribabu, S.-C. Ke, Int. J. Mol. Sci., 2023, 24(15), 11896. (IF: 6.92).
- Imidazole-based dual functional chemosensor for the recognition of Cu²⁺ and CN⁻: Applications in real water samples and colorimetric test strips
 M. Kumar, S. Munusamy, D. Jothi, S. Enbanathan, <u>J. Haribabu</u>, S. Kulathu Iyer, *Opt. Mater.*, 2023, 144, 114382. (IF: 3.75).
- Exploring the anticancer potential of thiadiazole derivatives of substituted thiosemicarbazones formed *via* copper-mediated cyclization
 V. P. V. Namboothiri, *J. Haribabu*, S.K. Vaishnu, M. Vipin, P. Rasin, N. Bhuvanesh, C. Echeverria, J.F. Santibanez, A. Sreekanth, *Appl. Organomet. Chem.*, 2023, e7174. (IF: 4.07).
- An active ESIPT based molecular sensor aided with sulfonate ester moiety to track the presence of H₂S analyte in realistic samples and HeLa cells
 V. Kavitha, P. Viswanathamurthi, <u>J. Haribabu</u>, E. Cesar, *Microchemical Journal*, 2023, 188, 108484 (IF: 5.30).
- 21. A new nitrile vinyl linked ultrafast receptor to track cyanide ions: Utilization on realistic samples and HeLa cell imaging
 V. Kavitha, P. Viswanathamurthi, *J. Haribabu*, E. Cesar, *Spectrochim. Acta A*, 2023, 295, 122607, (IF: 4.83).
- 22. A Reversible Fluorescent Chemosensor for the Selective Detection of Cu^{2+} and CN^{-} ions by Displacement Approach





P. Viswanathamurthi, R. Divya, V. Kavitha, <u>J. Haribabu</u>, E. Cesar, J. Fluoresc., 2023, doi: 10.1007/s10895-023-03381-2 (IF: 2.52).

- 23. Anti-proliferative potential of copper(I) acylthiourea complexes with triphenylphosphine against breast cancer cells
 D. P. Dorairaj, <u>J. Haribabu</u>, D. Mahendiran, R.E. Malekshah, S.C.N. Hsu, R. Karvembu, *Appl. Organomet. Chem.*, 2023, e7087, (IF: 4.07).
- 24. A "turn-on" fluorescent chemosensor for the meticulous detection of gallium(III) ion and its use in live cell imaging, logic gates and keypad locks
 P. Rasin, *J. Haribabu*, K. Kailas Mahipal, M. Vipin, V. P. V. Namboothiri, P. Vadakkedathu, C. Echeverria, A. Sreekanth, *J. Photochem. Photobiol. A: Chem.*, 2023, 437, 114493 (IF: 5.14).
- MOFs as Versatile Catalysts: Synthesis Strategies and Applications in Value-Added Compound Production
 R.E. Malekshah, M. Moharramnejad, S. Gharanli, M. Shahi, A. Ehsani, *J. Haribabu*, H. Ouachtak, B. Mirtamizdoust, M. Sillanpää, H. Erfani, *ACS Omega*, 2023, 8, 31600–31619 (IF: 4.13), Review article.
- A Simple Selective Probe for Lysine Detection in Tablets, Food Samples and Cells V. Kavitha, V. Snega, P. Viswanathamurthi, <u>J. Haribabu</u>, J. Fluoresc., 2023, doi: 10.1007/s10895-023-03523-6 (IF: 2.52).
- 27. An aqueous mediated ultrasensitive facile probe incorporated with acrylate moiety to monitor cysteine in food samples and live cells
 V. Kavitha, P. Viswanathamurthi, *J. Haribabu*, E. Cesar, *Spectrochim. Acta A*, 2023, 293, 122447, (IF: 4.83).
- 28. Synthesis, spectroscopic characterizations, single crystal X-ray analysis, DFT calculations, *in vitro* biological evaluation and in silico evaluation studies of thiosemicarbazones based 1,3,4-thiadiazoles

V. P. Vishnunarayanan Namboothiri, *J. Haribabu*, M. Vipin, P. Rasin, V. Roslin Elsa, D. Gayathri, N. Bhuvanesh, C. Echeverria, A. Sreekanth, *J. Mol. Struct.*, 2023, 1273, 134309 (IF: 3.84).

- Piano stool Ru(II)-arene complexes having three monodentate legs: A comprehensive review on their development as anticancer therapeutics over the past decade
 S. Swaminathan, *J. Haribabu*, N. Balakrishnan, P. Vasanthakumar, R. Karvembu, *Coordination Chemistry Reviews*, 2022, 457, 214403, (IF: 24.83), Review article.
- Design and synthesis of heterocyclic azole based bioactive compounds: Molecular structure, quantum simulation, and mechanistic studies through docking as multi-target inhibitors of SARS-CoV-2 and cytotoxicity
 J. Haribabu, V. Garisetti, R. E. Malekshah, S. Srividya, D. Gayathri, N. Bhuvanesh, R.V. Mangalaraja, C. Echeverria, R. Karvembu, J. Mol. Struct., 2022, 1250, 131782 (IF: 3.84).
- Design of a dual responsive receptor with oxochromane hydrazide moiety to monitor toxic Hg²⁺ and Cd²⁺ ions: Usage on real samples and live cells
 V. Kavitha, M. Ramya, P. Viswanathamurthi, *J. Haribabu*, C. Echeverria, *Environ. Pollut.*, 2022, 301, 119036 (IF: 9.98).



32. Coordination behaviour of acylthiourea ligands in their Ru(II)-benzene complexes – Structures and anticancer activity

UNIVERSIDAD DE ATACAMA

S. Swaminathan, <u>J. Haribabu</u>, M. K. M. Subarkhan, G. Manonmani, K. Senthilkumar, N. Balakrishanan, N. Bhuvanesh, C. Echeverria, R. Karvembu, *Organometallics*, 2022, 41, 1621–1630, (IF: 3.87).

- 33. Development of thiosemicarbazone-based transition metal complexes as homogeneous catalysts for various organic transformations
 S. Priyarega, *J. Haribabu*, R. Karvembu, *Inorganica Chim. Acta*, 2022, 532, 120742 (IF: 3.11) Review article.
- Pd(II)–PPh₃ complexes of halogen substituted acylthiourea ligands: Biomolecular interactions and anticancer activity
 D.P. Dorairaj, *J. Haribabu*, Y.L. Chang, C. Echeverria, S.C.N. Hsu, R. Karvembu, *Appl. Organomet. Chem.*, 2022, 36, e6765, (IF: 4.07).
- 35. Effect of *N*-benzyl group in indole scaffold of thiosemicarbazones on the biological activity of their Pd(II) complexes: DFT, biomolecular interactions, *in silico* docking, ADME and cytotoxicity studies

B. Nithya, *J. Haribabu*, R.E. Malekshah, S. Srividya, C. Balachandran, N. Bhuvanesh, S. Aoki, R. Karvembu, *Inorganica Chim. Acta*, 2022, 534, 120805 (IF: 3.11).

- Bidentate acylthiourea ligand-anchored Pd-PPh3 complexes with biomolecular binding, cytotoxic, antioxidant and anti-hemolytic properties
 D. P. Dorairaj, *J. Haribabu*, P.V.S. Shashankh, Y.-L. Chang, C. Echeverria, S.C. N. Hsu, R. Karvembu, *J. Inorg. Biochem.*, 2022, 233, 111843, (IF: 4.33).
- Impact of denticity of chromone / chromene thiosemicarbazones in the ruthenium(II)-DMSO complexes on their cytotoxicity against breast cancer cells
 N. Balakrishanan, <u>J. Haribabu</u>, D. Mahendiran, S. Swaminathan, R. Karvembu, *Appl. Organomet. Chem.*, 2022, 36, e6750, (IF: 4.07).
- 38. A new subtle and integrated detector to sense Hg²⁺ ions: A vision towards its applicability on water samples and live cells
 V. Kavitha, P. Viswanathamurthi, *J. Haribabu*, C. Echeverria, *J. Photochem. Photobiol. A: Chem.*, 2022, 428, 113863 (IF: 5.14).
- Flow injection analysis-based electrochemiluminescence: An overview of experimental design and its biosensing applications
 C. Venkateswara Raju, G. Mohana Rani, <u>J. Haribabu</u>, S. Senthil Kumar, ECS Sensors Plus, 2022, 1, 031604 (IF: 0. 521).
- 40. Synthesis, structural, DNA/protein binding and cytotoxic studies of copper(I) ∝-diimine hydrazone complexes
 S. Gayathri, P. Viswanathamurthi, V. Thuslim, M. Sathya, M. Ranjani, R. Prabhakaran, *J. Haribabu*, C. Echeverria, *Inorganica Chim. Acta*, 2022, 533, 120780 (IF: 3.11).
- 41. Simple fluorescence sensing approach for selective detection of Fe³⁺ Ion: Live cell imaging and logic gate functioning





P. Rasin, M. Vipin, V. P. Vishnunarayanan Namboothiri, <u>J. Haribabu</u>, E. Cesar, A. Sreekanth, ACS Omega, 2022, 7, 33248–33257 (IF: 4.13).

42. Dinitro dinitrobenzene ether reactive turn-on fluorescence probes for the selective detection of H_2S

R. Dhivya, V. Kavitha, A. Gomathi, P. Keerthana, N. Santhalakshmi, P. Viswanathamurthi, *J. Haribabu*, *Anal. Methods*, 2022, 14, 58-66 (IF: 3.53).

- 43. N-Substitution in isatin thiosemicarbazones decides nuclearity of Cu(II) complexes Spectroscopic, molecular docking and cytotoxic studies
 <u>J. Haribabu</u>, O.I. Alajrawy, K. Jeyalakshmi, C. Balachandran, D.A. Krishnan, N.S.P. Bhuvanesh, S. Aoki, K. Natarajan, R. Karvembu, *Spectrochim. Acta A*, 2021, 246, 118963 (12 pages) (IF: 4.83).
- 44. Synthesis, cytotoxicity, and docking studies (with SARS-CoV-2) of water-soluble binuclear Ru-*p*-cymene complex holding indole thiosemicarbazone ligand <u>J. Haribabu</u>, N. Balakrishnan, S. Swaminathan, P. Jerome, D. Gayathri, C. Echeverria, N. Bhuvanesh, R. Karvembu, *Inorg. Chem. Commun.*, 2021, 134, 109029 (IF: 2.71).
- 45. Synthesis and anticancer properties of bis- and mono(cationic peptide) hybrids of cyclometalated iridium(III) complexes: Effect of the number of peptide units on anticancer activity

J. Haribabu, Y. Tamura, K. Yokoi, C. Balachandran, M. Umezawa, K. Tsuchiya, Y. Yamada, R. Karvembu, S. Aoki, *Eur. J. Inorg. Chem.*, 2021, 1796-1814, (IF: 2.52). (Top cited paper 2022).

46. Impact of aliphatic acyl and aromatic thioamide substituents on the anticancer activity of Ru(II)*p*-cymene complexes carrying acylthiourea ligands – *In vitro* and *in vivo* studies

S. Swaminathan, <u>J. Haribabu</u>, M.K.M. Subarkhan, D. Gayathri, N. Balakrishnan, N. Bhuvanesh, C. Echeverria, R. Karvembu, *Dalton Trans.*, 2021, 50, 16311-16325 (IF: 4.39). (Top 10% of highly cited articles, 2022).

- 47. Tunable anticancer activity of furoylthiourea-based Ru(II)-arene complexes and their mechanism of actionS. Swaminathan, *J. Haribabu*, K. Naveen Kumar, N. Maroli, N. Balakrishnan, N. Bhuvanesh,
 - K. Kadirvelu, P. Kolandaivel, R. Karvembu, *Chem. Eur. J.*, 2021, 27, 7418-7433, (IF: 5.23).
- Effect of morphology and (Sn, Cr) doping on *in vitro* antiproliferation properties of hydrothermally synthesized 1D GaOOH nanostructures
 P. Rekha, *J. Haribabu*, M.K.M. Subarkhan, C. Echeverria, R. Karvembu, N. Gopalakrishnan, *J. Sci.: Adv. Mater. Dev.*, 2021, 6, 351-363, (IF: 7.38).
- Effect of new Pd(II)-aroylthiourea complex on pancreatic cancer cells
 D. P. Dorairaj, <u>J. Haribabu</u>, Y.L. Chang, S.C.N. Hsu, C. Echeverria, J. Echeverria, R. Karvembu, *Inorg. Chem. Commun.*, 2021, 134, 109018, (IF: 2.71).
- 50. Cyclometalated iridium(III)-cationic peptide hybrids trigger paraptosis in cancer cells *via* an intracellular Ca²⁺ overload from the endoplasmic reticulum and a decrease in mitochondrial membrane potential





C. Balachandran, K. Yokoi, K. Naito, <u>J. Haribabu</u>, Y. Tamura, M. Umezawa, K. Tsuchiya, T. Yoshihara, S. Tobita, S. Aoki, *Molecules*, 2021, 26, 7028 (IF: 4.41).

- Binding mode transformation and biological activity on the Ru(II)-DMSO complexes bearing heterocyclic pyrazolyl ligands
 D. Priyanka, L. Ya-Fan, *J. Haribabu*, M. Theetharappan, N. Manmath, R. Karvembu, M. Neelakantan, C. Chien-Chih, S.C.N. Hsu, *J. Inorg. Biochem.* 2021, 223, 111545, (IF: 4.15).
- 52. 2'-Thiophenecarboxaldehyde derived thiosemicarbazones metal complexes of copper(II), palladium(II) and zinc(II) ions: Synthesis, spectroscopic characterization, anticancer activity and DNA binding studies

M. Lavanya, *J. Haribabu*, K. Ramaiah, C. Suresh Yadav, C. Ramesh Kumar, J. Jang, R. Karvembu, A. Varada Reddy, M. Jagadeesh, *Inorganica Chim. Acta*, 2021, 524, 120440, (IF: 2.54).

Spectroscopic, anticancer and antioxidant studies of fluxional *trans*-[PdCl₂(S-acylthiourea)₂] complexes
 D. P. Dorairaj, *J. Haribabu*, V. Chithravel, K.N. Vennila, N. Bhuvanesh, C. Echeverria, S.C.

N. Hsu, R. Karvembu, *Results in Chem.*, 2021, 3, 100157.

- 54. Near-infrared fluorogenic receptor for selective detection of cysteine in blood serum and living cells
 A. Gomathi, P. Viswanthamurthi, *J. Haribabu*, *Anal. Bioanal. Chem.*, 2021, 413, 1817-1826 (IF: 4.14).
- Effective inhibition of insulin Amyloid fibril aggregation by nickel(II) complexes containing heterocyclic thiosemicarbazones
 K. Gomathi,^a J. Haribabu,^a S. Saranya, D. Gayathri, K. Jeyalakshmi, S. Sendilvelan, C. Echeverria, R. Karvembu, *Eur. Biophys. J*, 2021, 50, 1069-1081, (IF: 2.09) ^aEqual Contribution..
- 56. Synthesis of palladium(II) complexes *via* michael addition: Antiproliferative effects through ROS-mediated mitochondrial apoptosis, and docking with SARS-COV-2

J. Haribabu, S. Srividya, D. Mahendiran, D. Gayathri, V. Venkatramu, N. Bhuvanesh, R. Karvembu, *Inorg. Chem.*, 2020, 59, 17109-17122, (IF: 5.16).

Note: This article is made available via the ACS COVID-19 subset for unrestricted RESEARCH re-use and analyses in any form or by any means with acknowledgement of the original source. These permissions are granted for the duration of the World Health Organization (WHO) declaration of COVID-19 as a global pandemic.

- Thiosemicarbazone(s)-anchored water soluble mono- and bimetallic Cu(II) complexes: Enzymes-like activities, biomolecular interactions, anticancer property and real-time live apoptosis study
 B. Nithya, *J. Haribabu*, D. Anantha Krishnan, S. Srividya, S. Sun, D.F. Dibwe, N.S.P. Bhuvanesh, S. Awale, R. Karvembu, *Dalton Trans.*, 2020, 49, 9411-9424, (IF: 4.39).
- 58. Unprecedented formation of palladium(II)-pyrazole based thiourea from chromone thiosemicarbazone and [PdCl₂(PPh₃)₂]: Interaction with biomolecules and apoptosis by the complexes through mitochondrial signaling pathway





J. Haribabu, C. Balachandran, M. Muthu Tamizh, Y. Arun, N.S.P. Bhuvanesh, S. Aoki, R. Karvembu, J. Inorg. Biochem., 2020, 205, 110988, (IF: 4.15).

- 59. Enhanced anticancer activity of half-sandwich Ru(II)-*p*-cymene complex bearing heterocyclic hydrazone ligand
 <u>J. Haribabu</u>, S. Srividya, R. Umapathi, D. Gayathri, P. Venkatesu, N. Bhuvanesh, R. Karvembu, *Inorg. Chem. Commun.*, 2020, 119, 108054, (IF: 2.49).
- Pd(II)-NNN pincer complexes for catalyzing transfer hydrogenation of ketones
 P. Jerome, *J. Haribabu*, N.S.P. Bhuvanesh, R. Karvembu, *ChemistrySelect*, 2020, 5, 13591-13597, (IF: 2.10).
- 61. Half-sandwich Ru-(η^6 -*p*-cymene) complexes featuring pyrazol appended ligands: Synthesis, DNA binding and *in vitro* cytotoxicity

Y.C. Huang,^a <u>J. Haribabu,^a</u> C.M. Chien, G. Sabapathi, C.K. Chou, R. Karvembu, P. Venuvanalingam, W.M. Ching, M.L. Tsai, S.C.N. Hsu, J. Inorg. Biochem., 2019, 194, 74-84, (IF: 3.22), ^aEqual Contribution.

- 62. Water-soluble mono- and binuclear Ru(η⁶-p-cymene) complexes containing indole thiosemicarbazones: Synthesis, DFT modeling, biomolecular interactions and *in vitro* anticancer activity through apoptosis
 J. Haribabu, G. Sabapathi, M.M. Tamizh, C. Balachandran, N.S.P. Bhuvanesh, P. Venuvanalingam, R. Karvembu, Organometallics, 2018, 37, 1242-1257, (IF: 4.10).
- Coordination behavior of N,N',N"-trisubstituted guanidine ligands in their Ru-arene complexes: Synthetic, DNA/protein binding, and cytotoxic studies
 K. Jeyalakshmi, <u>J. Haribabu</u>, C. Balachandran, S. Srividya, N. Bhuvanesh, R. Karvembu, Organometallics, 2019, 38, 753-770, (IF: 4.10).
- NHC catalyzed green synthesis of functionalized chromones: DFT mechanistic insights and *in vitro* activities in cancer cells
 N. Murugesh, *J. Haribabu*, K. Arumugam, C. Balachandran, R. Swaathy, S. Aoki, A. Sreekanth, R. Karvembu, S. Vedachalam, *New J. Chem.*, 2019, 43, 13509-13525, (IF: 3.06).
- Molecular structures, Hirshfeld analysis and biological investigations of isatin based thiosemicarbazones
 S. Saranya, ^a J. Haribabu, ^a V.N.V. Palakkeezhillam, P. Jerome, K. Gomathi, K.K. Rao, V.H.H. Surendra Babu, R. Karvembu, D. Gayathri, J. Mol. Struct., 2019, 1198, 126904, (IF: 2.12), ^aEqual Contribution.
- 66. Synthesis and anticancer activity of [RuCl₂(η⁶-arene)(aroylthiourea)] complexes High activity against human neuroblastoma (IMR-32) cancer cells
 S. Srividya, *J. Haribabu*, B. Nithya, K. Ramaiah, C. Balachandran, N. Bhuvanesh, R. Karvembu, *ACS Omega*, 2019, 4, 6245-6256, (IF: 2.58).
- Synthesis and molecular structure of zinc(II) complex bearing N, S donor ligand <u>J. Haribabu</u>, S. Priyarega, N.S.P. Bhuvanesh, R. Karvembu, J. Struct. Chem., 2020, 61, 71-77, (IF: 1.07).



 Design, synthesis, DNA/HSA binding and cytotoxic activity of half-sandwich Ru(II)-arene complexes containing triarylamines-thiosemicarbazone hybrids M. Muralisankar, R. Dheepika, <u>J. Haribabu</u>, C. Balachandran, S. Aoki, N.S.P. Bhuvanesh, S. Nagarajan, *ACS Omega*, 2019, 4, 11712-11723, (IF: 2.58).

- Highly active copper(I) complexes of aroylthiourea ligands against cancer cells Synthetic and biological studies
 K, Jeyalakshmi, <u>J. Haribabu</u>, C. Balachandran, E. Narmatha, N.S.P. Bhuvanesh, S. Aoki, R. Karvembu, *New J. Chem.*, 2019, 43, 3188-3198, (IF: 3.06).
- 70. Zinc(II) complexes of indole thiosemicarbazones: DNA/protein binding, molecular docking and *in vitro* cytotoxicity studies
 B. Nithya, *J. Haribabu*, D. Anantha Krishnan, S. Srividya, D. Mahendiran, N.S.P. Bhuvanesh, R. Karvembu, *Polyhedron*, 2019, 170, 188-201, (IF: 2.06).
- Chemosensing, molecular docking and antioxidant studies of 8-amino quinoline appended acylthiourea derivatives
 A. Kalaiyarasi, <u>J. Haribabu</u>, K. Gomathi, D. Gayathri, N.S.P. Bhuvanesh, R. Karvembu, V.M. Biju, J. Mol. Struct., 2019, 1185, 450-460, (IF: 2.12).
- 72. Effect of 2-bromopyridine ancillary ligand in the catalysis of Pd(II)-NNN pincer complexes towards Suzuki-Miyaura cross-coupling reaction
 P. Jerome, S.Yasar Arafath, *J. Haribabu*, N.S.P. Bhuvanesh, R. Karvembu, *ChemistrySelect*, 2019, 4, 2237-2241, (IF: 1.71).
- Vibrational spectroscopic (FT-IR, FT-Raman), anti-inflammatory, docking and molecular characteristic studies of Ni(II) complex of 2-aminonicotinaldehyde using theoretical and experimental methods
 K. Ramaiah, J. Prashanth, *J. Haribabu*, E. Srikanth, B. Venkatram Reddy, R. Karvembu, K.L. Reddy, *J. Mol. Struct.*, 2019, 1175, 769-781, (IF: 2.12).
- 74. Synthesis, structures and mechanistic pathways of anticancer activity of palladium(II)complexes with indole-3-carbaldehyde thiosemicarbazones
 <u>J. Haribabu</u>, M.M. Tamizh, C. Balachandran, Y. Arun, N.S.P. Bhuvanesh, A. Endo, R. Karvembu, *New J. Chem.*, 2018, 42, 10818-10832, (IF: 3.06).
- 75. Nickel(II) bis(isatin thiosemicarbazone) complexes induced apoptosis through mitochondrial signaling pathway and G0/G1 cell cycle arrest in IM-9 cells
 C. Balachandran,^a J. Haribabu,^a K. Jeyalakshmi, N.S.P. Bhuvanesh, R. Karvembu, N. Emi, S. Awale, J. Inorg. Biochem., 2018, 182, 208-221, (IF: 3.22), ^aEqual Contribution.
- 76. Synthesis, structural, biological evaluation, molecular docking and DFT studies of Co(II), Ni(II), Cu(II), Cn(II), Cd(II) and Hg(II) complexes bearing heterocyclic thiosemicarbazone ligand K. Ramaiah, <u>J. Haribabu</u>, J. Prashanth, N.B. Venkata, M. Ramachary, G. Durgaiah, R. Karvembu, B.V. Reddy, Y.N. Reddy, K.L. Reddy, *Appl. Organom. Chem.*, 2018, 32, e4415, (IF: 3.58).



77. Ru(II)-η⁶-arene complexes of dibenzosuberenyl appended aroyl/acylthiourea ligands: *In vitro* biomolecular interaction studies and catalytic transfer hydrogenation
G. Rohini, *J. Haribabu*, M.M. Sheeba, K.N. Anees Rahman, N.S.P. Bhuvanesh, C. Balachandran, R. Karvembu, A. Sreekanth, *ChemistrySelect*, 2018, 3, 18-28, (IF: 1.71).

- 78. Synthesis, crystal structure, DNA binding and antitumor studies of β-diketonate complexes of divalent copper, zinc and palladium
 M. Lavanya, M. Jagadeesh, *J. Haribabu*, R. Karvembu, H.K. Rashmi, P.U.M. Devi, A. Varada Reddy, *Inorganica Chim. Acta*, 2018, 469, 76-86, (IF: 2.43). (Top cited paper 2019)
- 79. Half-sandwich Ru(II)(η⁶-*p*-cymene) complexes bearing *N*-dibenzosuberenyl appended thiourea for catalytic transfer hydrogenation and *in vitro* anticancer activity
 G. Rohini, <u>J. Haribabu</u>, K.N. Anees Rahman, R. Konakanchi, N.S.P. Bhuvanesh, R. Karvembu, A. Sreekanth, *Polyhedron*, 2018, 152, 147-154, (IF: 2.06) Review article.
- Synthesis of Ni(II) complexes bearing indole-based thiosemicarbazone ligands for interaction with biomolecules and some biological applications
 J. Haribabu, K. Jeyalakshmi, Y. Arun, N.S.P. Bhuvanesh, P.T. Perumal, R. Karvembu, J. Biol. Inorg. Chem., 2017, 22, 461-480, (IF: 3.63).
- 81. Ru(II)-*p*-cymene thiosemicarbazone complexes as inhibitors of Amyloid β (Aβ) peptide aggregation and Aβ-induced cytotoxicity
 J. Haribabu, D.S. Ranade, N.S.P. Bhuvanesh, P.P. Kulkarni, R. Karvembu, *ChemistrySelect*, 2017, 2, 11638-11644, (IF: 1.71).
- Synthesis of Ru(II)-benzene complexes containing aroylthiourea ligand, and their binding with biomolecules and *in vitro* cytotoxicity through apoptosis
 K. Jeyalakshmi, *J. Haribabu*, C. Balachandran, N.S.P. Bhuvanesh, N. Emi, R. Karvembu, *New J. Chem.*, 2017, 41, 2672-2686, (IF: 3.06).
- Copper, nickel and zinc complexes of 3-acetyl coumarin thiosemicarbazone: Synthesis, characterization and *in vitro* evaluation of cytotoxicity and DNA/protein binding properties K.N. Anees Rahman, <u>J. Haribabu</u>, C. Balachandran, N.S.P. Bhuvanesh, R. Karvembu, A. Sreekanth, *Polyhedron*, 2017, 135, 26-35, (IF: 2.28).
- In vitro antioxidant, anti-inflammatory and *in silico* molecular docking studies of thiosemicarbazones
 G.R. Subhashree,^a J. Haribabu,^a S. Saranya, P. Yuvaraj, D.A. Krishnan, R. Karvembu, D. Gayathri, J. Mol. Struct., 2017, 1145, 160-169, (IF: 2.12), ^aEqual Contribution.
- An investigation on the DNA/protein binding, DNA cleavage and *in vitro* anticancer properties of SNO pincer type palladium(II) complexes with *N*-substituted isatin thiosemicarbazone ligands
 M. Muralisankar, M.B. Sabeel, *J. Haribabu*, N.S.P. Bhuvanesh, R. Karvembu, A. Sreekanth, *Inorganica Chim. Acta*, 2017, 466, 61-70, (IF: 2.43).
- 86. Naphthalenyl appended semicarbazone as "turn on" fluorescent chemosensor for selective recognition of fluoride ion





M.B. Sabeel, *J. Haribabu*, N.S.P. Bhuvanesh, R. Karvembu, A. Sreekanth, *J. Mol. Struct.*, 2017, 1145, 347-355, (IF: 2.12).

- 87. Half-sandwich RuCl₂(η⁶-*p*-cymene) core complexes containing sulfur donor aroylthiourea ligand: DNA and protein binding, DNA cleavage and cytotoxic studies
 K. Jeyalakshmi, *J. Haribabu*, N.S.P. Bhuvanesh, R. Karvembu, *Dalton Trans.*, 2016, 45, 12518-12531, (IF: 4.05).
- Isatin based thiosemicarbazone derivatives as potential bioactive agents: Anti-oxidant and molecular docking studies
 J. Haribabu, G.R. Subhashree, S. Saranya, K. Gomathi, R. Karvembu, D. Gayathri, J. Mol. Struct., 2016, 1110, 185-195, (IF: 2.12).
- Synthesis, X-ray crystal structure, DNA/protein binding, DNA cleavage and cytotoxicity studies of N(4) substituted thiosemicarbazone based copper(II)/nickel(II) complexes M. Muralisankar, *J. Haribabu*, N.S.P. Bhuvanesh, R. Karvembu, A. Sreekanth, *Inorganica Chim. Acta*, 2016, 449, 82-95, (IF: 2.43).
- Synthesis, DNA/protein binding, molecular docking, DNA cleavage and *in vitro* anticancer activity of nickel(II) *bis*(thiosemicarbazone) complexes
 J. Haribabu, K. Jeyalakshmi, Y. Arun, N.S.P. Bhuvanesh, P.T. Perumal, R. Karvembu, RSC Adv., 2015, 5(57), 46031-46049, (IF: 3.04).
- 91. Synthesis, crystal structure, and *in vitro* and *in silico* molecular docking of novel acyl thiourea derivatives
 J. Haribabu, G.R. Subhashree, S. Saranya, K. Gomathi, R. Karvembu, D. Gayathri, J. Mol. Struct., 2015, 1094, 281-291, (IF: 2.12).
- 92. Facile and diastereo selective synthesis of 3,2'-spiropyrrolidine-oxindoles derivatives, their molecular docking and antiproliferative activities
 D. Kathirvelan, *J. Haribabu*, B.S.R. Reddy, C. Balachandran, V. Duraipandiyan, *Bioorganic Med. Chem. Lett.*, 2015, 25, 389-399, (IF: 2.44).
- 93. A facile and diastereoselective synthesis of functionalized spirooxindoles *via* 3+2 cycloaddition reaction
 D. Kathiruolon, I. Haribahu, P.S.P. Paddy, Indian I. Cham. 2015, 54P, 065, 071 (IE: 0.50).

D. Kathirvelan, J. Haribabu, B.S.R. Reddy, Indian J. Chem., 2015, 54B, 965-971, (IF: 0.50).

STRUCTURE REPORTS

- 94. 1'-(1,3-Diphenyl-1*H*-pyrazol-4-yl)-1"-methyl2',3',5',6',7',7a'octahydro1'*H*-dispiro[1-benzopyran -3,2'-pyrrolizine-3',3"-indoline]-2",4 dione
 G. Jagadeesan, K. Sethusankar, D. Kathirvelan, *J. Haribabu*, B.S.R. Reddy, *Acta Cryst.*, 2013, E69, o317.
- 95. (6'*R**,7'*R**)-7'-(1,3,-Diphenyl-1*H*-pyrazol-4-yl)-1,2,5',6',7',7a',3",4'octahydro1'*H*,2"*H*dispiro [acenaphthylene-1,5'-pyrrolo[1,2-*c*][1,3]thiazole-6',3"-[1]benzopyran]-2,4"-dione





J. Murugan, <u>J. Haribabu</u>, B.S.R. Reddy, G. Rajarajan, S. Murugavel, Acta Cryst., 2013, E69, 0493-0494.

- 96. 1'-(1,3-Diphenyl-1H-pyrazol-4-yl)-2',3',5',6',7',7a'-hexa-hydro-1'H-di-spiro-[ace-naphthyl-ene-1,3'-pyrrolizine-2',3"-chromane]-2,4"(1H)-dione G. Jagadeesan, D. Kathirvelan, *J. Haribabu*, B.S.R. Reddy, K. Sethusankar, *Acta Cryst.*, 2013, E69, o711.
- 97. 1'-(1,3-Diphenyl-1H-pyrazol-4-yl)-1"-(prop-2-en-1-yl)-2',3',5',6',7',7a'-hexahydro-1'Hdispiro [1-benzopyran-3,2'-pyrrolizine-3',3"-indoline]-2",4-dione 0.75-hydrate G. Jagadeesan, D. Kathirvelan, *J. Haribabu*, B.S.R. Reddy, K. Sethusankar, *Acta Cryst.*, 2013, E69, o1194-o1195.
- 98. Crystal structure of (2E)-*N*-methyl-2-[(4-oxo-4H-chromen-3-yl)methylidene]hydrazine-carbothioamide
 G. Vimala, J. Govindaraj, <u>J. Haribabu</u>, R. Karvembu, A. Subbiah Pandi, *Acta Cryst.*, 2014, E70(11), o1151.
- 99. Crystal structure of (E)-2-[(4-chloro-2H-chromen-3-yl)methylidene]-*N*-cyclohexylhydrazine carbothioamide

R. Gangadharan, <u>J. Haribabu</u>, R. Karvembu, K. Sethusankar, Acta Cryst., 2014, E70(9), o1039-o1040.

- 100. Crystal structure of (2*E*)-*N*-methyl-2-(2-oxo-1,2-di-hydroacenaphthylen-1-ylidene) hydrazine carbothio amide
 G. Vimala, J. Govindaraj, *J. Haribabu*, R. Karvembu, A. Subbiah Pandi, *Acta Cryst. (Research Communications)*, 2014, 70(11), 415-417.
- 101. Crystal structure of *N*-[(4-ethoxyphenyl)carbamothioyl]cyclohexanecarboxamide
 G. Vimala, *J. Haribabu*, S. Srividya, R. Karvembu, A. Subbiah Pandi, *Acta Cryst.*, 2015, E71(10), o820-o821.
- 102. Crystal structure of *N*-[(naphthalen-1-yl)carbamothioyl]cyclohexanecarboxamide
 G. Vimala, *J. Haribabu*, S. Aishwarya, R. Karvembu, A. Subbiah Pandi, *Acta Cryst.*, 2015, E71(7), o508-o509.
- 103. Crystal structures of two hydrazinecarbothioamide derivatives: (E)-*N*-ethyl-2-((4-oxo-4H-chromen-3-yl) methylene) hydrazinecarbothioamidehemihydrate and (E)-2-((4-chloro-2H-chromen-3-yl)methylidene)-*N*-phenyl hydrazinecarbothioamide
 R. Gangadharan, <u>J. Haribabu</u>, R. Karvembu, K. Sethusankar, *Acta Cryst. (Research Communications)*, 2015, 71(3), 305-308.
- 104. Crystal structure of (Z)-2-(1-benzyl-2-oxoindolin-3-ylidene)-*N*-phenylhydrazine-1-carbo thioamide
 G. Vimala, *J. Haribabu*, R. Karvembu, B.V.N.P. Kumar, A. Subbiah Pandi, *Acta Cryst.*, 2015, 71(3), 0160-0161.
- 105. Crystal structures of the Schiff base derivatives (E)-*N*'-[(1H-indol-3-yl)methylidene]isonicotinohydr- azide ethanol monosolvate and (E)-*N*-methyl-2-[1-(2-oxo-2H-chromen-3-yl)ethylidene]hydrazinecarbo- thioamide

S. Saranya, *J. Haribabu*, N.S.P. Bhuvanesh, R. Karvembu, D. Gayathri, *Acta Cryst. (Research Communications)*, 2017, 73(4), 594-597.





LIST OF BOOK

 Biomolecular interactions, and anticancer activity of Ni, Pd and Ru complexes bearing heterocyclic thiosemicarbazone ligands – Book
 J. Haribabu, K. Jeyalakshmi, R. Karvembu, Lambert Academic Publishing (<u>https://www.lap-publishing.com/</u>), Germany, 2020, ISBN-13: 978-620-4-19015-0, ISBN-10:6204190156, EAN:9786204190150 (392 pages).

LIST OF BOOK CHAPTERS

Polymer-ceramic based solid composite membranes as potential electrolytes for the lithium batteries – Book Chapter 9 (Advanced Ceramics for Versatile Interdisciplinary Applications)
 G. Mohana Rani, P. Rawat, <u>J. Haribabu</u>, P. Ranjan Sahoo, R. Kumar, R. Umapathi, Elsevier, Book Chapter 9, 2021, ISBN: 9780323899529, 182-200 (https://www.elsevier.com/books/advanced-ceramics-for-versatile-interdisciplinary-applications/singh/978-0-323-89952-9).

REVISED AND UNDER REVIEW MANUSCRIPTS

- Pernicious effect of hydrothermally synthesized pure, Sn doped and Cr doped β-Ga₂O₃ on cultured cancer cells
 P. Rekha, <u>J. Haribabu</u>, M.K.M. Subarkhan, A. Arulraj, R.V. Mangalaraja, E. Cesar, R. R. Tagle, N. Gopalakrishnan, *Materials Today Communications*, (Under Review), (IF: 3.66).
- Recent advances in silver nanoparticles-based approaches for colorimetric sensing of pesticides in water and food matrices
 R. Singh, *J. Haribabu*, H. Kumar, V. Kakani, N. Kumar, *Environ. Sci. Pollut. Res.*, (Under Review), (IF: 5.10).
- MOFs as Versatile Catalysts: Synthesis Strategies and Applications in Value-Added Compound Production
 S. Gharanli, R.E. Malekshah, M. Moharramnejad, M. Shahi, A.H. Joshaghani, A.H. Amini, <u>J.</u> *Haribabu*, E. Salih, *Coordination Chemistry Reviews*, (Under Review), (IF: 24.19).
- 4. Exploration of biological activity of cyclohexyl-based acylthiourea derivatives using theoretical means and MTT assay

G. Madhavana, S. Swaminathan, <u>J. Haribabu</u>*, M. Azamd, J. Petere, G. Dasararajua, J. Santibanez, M.J. Gallardo-Nelsonc, R.R. Tagle, *Int. J. Mol. Sci.*, (Under Review), (IF: 6.12). Corresponding Author.





INVITED LECTURES

- Invited talk on "First report on the synthesis of chromone-based Pd(II) complexes via Michael addition for Anticancer activity via apoptosis and multi-target inhibitors of SARS-CoV-2" at Departamento de Química de los Materiales, Universidad de Santiago de Chile, Santiago, Chile on 03 January 2024.
- 2. Invited talk on "Organometallic drugs with potential for the treatment of cancers (Fármacos organometálicos con potencial para el tratamiento del cáncer)" at Congerso Futuro, Centro Cultural Atacama Alameda Antonio Matta, Copiapo, Chile on 17th January 2024.
- 3. Invited talk on "First report on synthesis of Pd(II) complexes via Michael addition: Anticancer activity via apoptosis and mechanistic studies through docking as multi-target inhibitors of SARS-CoV-2" at XLIV Congreso Anual, Universidad Católica del Norte, Sede Antofagasta, Antofagasta, Chile. 04 y 07 de Diciembre del 2023.
- 4. Invited talk on "Awareness to College Students about Cancer and How Lifestyle Will Prevent Cancer?? Or Concientización a los estudiantes universitarios sobre el cáncer y cómo el estilo de vida prevenirá el cáncer??" at Colegio San Agustín de Atacama, Copiapó, Chile, 29/11/2022.
- Seven-day International Virtual Faculty Development Programme on Emerging Trends in Chemical Sciences (ETCS-2023) organised by the PG & Research Department of Chemistry, Seethalakshmi Ramaswami College, Tiruchirappalli, Tamil Nadu, India from 19.11.2023 to 25.11.2023 – "Development of Novel Metallodrugs for Anticancer and Antiviral Applications?" (Online).
- 6. Invited talk on "*Innovative Biofunctionalized Metal Complexes for Biological Applications*" at Vellore Institute of Technology, Vellore, Tamil Nadu, India, 28/09/2022.
- 7. Invited talk on "*How to Prevent Cancer Naturally?*" at Govt. Degree College, Vedurukuppam, Andhra Pradesh, India, 27/09/2022.
- 8. Invited talk on "*Can a Health Lifestyles Avoid Cancer?*" at Govt. Degree College, Nagari, Andhra Pradesh, India, 13/09/2022.
- 9. Invited talk on "Awareness about Cancer and Corona disease for Students, and Motivation towards Higher Education" at Sri Padmavathi Womens Degree College, Tirupati, Andhra Pradesh, India, 18/07/2022.
- 10. Invited talk on "*Cancer is Danger Disease?*" at Sri Venkateswara Arts College (TTD), Tirupati, Andhra Pradesh, India, 07/07/2022.
- Six Days International Faculty Development Program titled Innovative Trends in Science & Technology, M.Kumarasamy College of Engineering, Karur, India, 26-31/07/2021 –





"Organometallic (Ir and Ru) Compounds: Next-Generation Anticancer and Antiviral Metallodrugs?" (Online).

- 12. Science Dialogue Program, Utsunomiya Girls' High School, Utsunomiya, Tochigi, Japan, 26/10/2019 "Idea of Cancer and Anticancer Drugs, and Motivation of Students Towards to Research".
- 13. Novel Materials for Energy and Biological (COVID-19) Health Applications, M.Kumarasamy College of Engineering, Karur, India, 16/05/2020 – "Synthesis of Palladium(II) Complexes and Docking with SARS COV-2" (Online).
- 14. International Webinar for Engineering and Science, National Engineering College, Kovilpatti, India, 11/06/2020 – "Role of Engineers in Drug Design: Molecular Docking Studies" (Online).
- 15. **Innovative Strategies in Chemical Science and Technology (ISCST-2020)**, Bhaktavatsalam Memorial College for Women, India, 28/06/2020 "Design and Development of Novel Metal Complexes for Cancer Therapy" (Online).

ORAL PRESENTATIONS IN CONFERENCES

- 1. 64th Annual Meeting of the Pharmaceutical Society of Japan, Kanto Region, Japan, 19/09/2020 "Design, Synthesis and Anticancer Properties of Bis-, and Mono(Cationic Peptide) Hybrids of Ir(III) Complexes: Effect of the Number of Peptide Units on Anticancer Activity".
- 2. 7th International Postgraduate Conference on Pharmaceutical Sciences (iPoPS2020), Tokyo University of Science, Japan, 28/02/2020 – "Design, Synthesis, Bioimaging and Anticancer Properties of Mono-, and Disubstituted Cyclometalted Ir(III) Complex-Peptide Hybrids".
- 3. **3rd Acian Conference on Chemosensors and Imaging Probes (Asian ChIP-2019),** Guru Nanak Dev University, Amritsar, India, 06-09/11/2019 "Design and Synthesis of Cyclometalated Iridium(III) Complexes Based on Post Complexation Functionalization".
- 4. The 27th International Society of Heterocyclic Chemistry'' Congress (ISHC2019), ROHM Theatre Kyoto, Japan, 01-06/9/2019 – "Selective Substitution and Decomposition Reactions of Cyclometalated Iridium Complexes and Their Applications to Biomedical and Material Sciences".
- 5. International Conference on Synthetic Materials for Science and Engineering Applications (SMSEA-2018), M.Kumarasamy College of Engineering, Karur, India, 11/04/2018 "Formation of Pd(II)-pyrazole based thiourea from chromone thiosemicarbazone Apoptosis by the complexes".
- 6. **Research Awards,** Dr. K. V. Rao Scientific Society, Hyderabad, India, 27/05/2017 "Unprecedented formation of Pd(II)-pyrazole based thiourea from chromone thiosemicarbazone and [PdCl₂(PPh₃)₂]: Complexes induced apoptosis through mitochondrial signaling pathway and G0/G1 cell cycle arrest in HepG2 cells".



- 7. **3rd International Conference on Science**, Engineering and Technology (SET), Vellore Institute of Technology (VIT), Vellore, India, 17-18/02/2012 "Synthesis of novel spiro heterocyclic compounds from 1,3 dipolar cyclo-addition and biological studies".
- 8. 2nd International Conference on Science, Engineering and Technology (SET), Vellore Institute of Technology (VIT), Vellore, India, 20-21/04/2011 "Studies on synthesis of bis indoles and biological applications".
- 9. **25th National Science Day (NSD),** Vellore Institute of Technology (VIT), Vellore, India, 28/02/2011 "Solvent free synthesis of 1,3,5-trisubstituted pyrozolines using imidazolium based ionic liquid as solvent & catalyst: A green route approach".

CONFERENCES (POSTER PRESENTATIONS AND PARTICIPATED)

- C. Echeverría, D. Oyarzun, C. Monardes-Carvajal, S. Sanchez-Varas, I. Montorfano, J. Haribabu, The tricarbonyl rhenium(I) complexes and its potential use as an anticancer nanomedicine, XXXV Annual Meeting of the Society of Cellular Biology of Chile, Puerto Varas, Chile, 06-10/11/2023 (Poster Presentation).
- 2. D. Juan Muena, A. Soliz, **J. Haribabu**, Study of hydrogen generation with a electrode modified by "click chemistry" anchored with a Co(II) and Ni(II) porphyrin, XXI International Congress of Metallurgy and Materials, Viña del Mar, Chile, 05-10/11/2023 (Poster Presentation).
- 3. **J. Haribabu**, International year of chemistry (Chemistry Quiz by IYC Kalpakkam), Vellore Institute of Technology (VIT), Vellore, India, 15/09/2011 (Participated).
- 4. **J. Haribabu**, Chennai Chemistry Conference, CSIR-Central Leather Research Institute (CLRI), Chennai, India, 08-10/02/2013 (Participated).
- 5. J. Haribabu, New Avenues in Chemical Science Research (One-week short term course), National Institute of Technology (NIT), Trichy, India, 18-22/03/2013 (Participated).
- 6. **J. Haribabu**, Role of Inorganic Compounds in Medicine, National Institute of Technology (NIT), Trichy, India, 18/10/2013 (Participated).
- 7. J. Haribabu, National Conference on Chemosensores (NCC), National Institute of Technology (NIT), Trichy, India, 19-20/09/2013 (Participated).
- 8. J. Haribabu, Role of Inorganic Compounds in Medicine, National Institute of Technology (NIT), Trichy, India, 18/10/2013 (Participated).
- 9. J. Haribabu, R. Karvembu, Crystal structure of (E)-2-[(4-chloro-2H-chromen-3-yl) methylidene]-N-cyclohexylhydrazinecarbothioamide, National Conference on resent trends in X-ray crystallography, Seethalakshmi Ramaswami College, Trichy, India, 08-09/09/2014 (Poster Presentation).
- 10. **J. Haribabu**, Bio-Mimetic and Molecular Modeling, National Institute of Technology (NIT), Trichy, India, 11/01/2014 (Participated).



11. **J. Haribabu**, Innovation Methods in Chemical Science (One-week short term course), National Institute of Technology (NIT), Trichy, India, 05-09/05/2014 (Participated).

- 12. **J. Haribabu** and R. Karvembu, Novel water soluble organobimetallic Ru(II) complexes containing indole based thiosemicarbazone ligands: Synthesis, structure and *in vitro* biological evaluation, 17th CRSI National Symposium in Chemistry, National Chemical Laboratory (NCL), Pune, India, 06-08/02/2015 (Poster Presentation).
- 13. J. Haribabu, and R. Karvembu, Synthesis, DNA/protein binding, molecular docking, DNA cleavage and in vitro anticancer activity of nickel(II) bis(thiosemicarbazone) complexes, 10th Mid-Year CRSI Symposium in Chemistry, National Institute of Technology (NIT), Trichy, India, 23-25/07/2015 (Poster Presentation and Conference Organizer Member).
- 14. J. Haribabu, National level Symposium on Bio-Mimetic and Molecular Modeling, National Institute of Technology (NIT), Trichy, India, 12-13/09/2014 (Participated).
- 15. J. Haribabu, Innovative Catalysis, National Institute of Technology (NIT), Trichy, India, 11-12/09/2015 (Participated).
- 16. J. Haribabu, and R. Karvembu, Nickel(II) complexes with indole based thiosemicarbazone ligands for biological applications, Sixth International Conference on Metals in Genetics, Chemical Biology and Therapeutics, Indian Institute of Science (IISc), Bangalore, India, 17-20/02/2016 (Poster Presentation).
- 17. J. Haribabu, 19th National Convention of Electrochemists, National Institute of Technology (NIT), Trichy, India, 28-29/03/2016 (Participated).
- J. Haribabu, Workshop on Electronic Structure of Coordination Complexes, Indian Institute of Technology (IIT), Bombay, India, 16-18/05/2016 (Participated).
- 19. J. Haribabu, RSC-NIT Symposium on Heterogeneous Catalysis and Sustainable Chemistry, National Institute of Technology (NIT), Trichy, India, 28/05/2016 (Participated).
- 20. J. Haribabu, Novelistic Nanotechnology What Chemistry Behind it?, National Institute of Technology (NIT), Trichy, India, 16-17/09/2016 (Participated).
- 21. **J. Haribabu,** and R. Karvembu, Unprecedented formation of Pd(II)-pyrazole based thiourea from chromone thiosemi-carbazone and [PdCl₂(PPh₃)₂]-Apoptosis by the complexes through mitochondrial signaling pathway, 5th Symposium on Advanced Biological Inorganic Chemistry organized by TIFR, Mumbai and IACS, Jadavpur at Kolkata, India, 07-11/01/2017 (Poster Presentation).
- 22. J. Haribabu, Taiwan Bioinorganic Chemistry Society, National Chiayi University, Taiwan, 19/12/2017 (Participated).



- 23. **J. Haribabu,** S.C.N. Hsu, R. Karvembu, An investigation on DNA binding and in vitro anticancer properties of organometallics Ru(II)-(η^6 -*p*-cymene) complexes containing pyrazole based ligands, Republic of China biomedical materials and drug system society, Kaohsiung Medical University, Taiwan, 23/03/2018 (Poster Presentation).
- 24. A. Kalaiyarasi, **J. Haribabu**, R. Karvembu, V.M. Biju, Synthesis, characterization and molecular docking studies of 8-aminoquinoline appended thiourea compounds, Indian Analytical Science Congress, Mahatma Gandhi University, Kottayam, India, 08-10/02/2018 (Poster Presentation).
- 25. S.S. Ma, **J. Haribabu**, S.C.N. Hsu, The coordination behavior of 2-(3-pyrazoly) pyridine ligand on the Ru(II) complexes: From Monodentate to bidentate binding mode changes, Chinese Chemistry Conference, National Sun Yat-Sen University, Taiwan, 08/12/2018 (Poster Presentation).
- 26. J. Haribabu, K. Yokoi, Y. Tamura, C. Balachandran, S. Aoki, Design, Synthesis and Anticancer Activity of Bis-, and Mono(Cationic Peptide) Hybrids of Cyclometalated Iridium(III) Complexes: Effect of the Number of Peptide Units on Anticancer Property, The 70th Conference of Japan Society of Coordination Chemistry, Ibaraki University, Japan, 28-30/09/2020 (Poster Presentation).
- 27. J. Haribabu, Molecules-Future Trends in Bioorganic Chemistry, Switzerland, 01/06/2021 (Webinar- Participated).
- J. Haribabu, Science, technology and applications of rare earth metals' (STAR-2022), Departments of Physics and Chemistry at Sri Venkateswara University, Tirupati, India 22-23/09/2022 (Participated).
- J. Haribabu, Artificial Photosynthesis, RSC Desktop Seminars, London, 12/09/2023 (Webinar-Participated).

REFERENCES

- Dr. R. Karvembu (Ph.D. Supervisor) Professor of Chemistry National Institute of Technology Trichy-620015, Tamil Nadu India E-mail: <u>kar@nitt.edu</u> Mobile No: +91 94422 68653
- Dr. Sodio C. N. Hsu (Intern Supervisor) Professor of Medicinal and Applied Chemistry, Kaohsiung Medical University Kaohsiung 807, Taiwan E-mail: sodiohsu@kmu.edu.tw Tel No: +886-7-3121101, ext.6984





- Dr. Shin Aoki (JSPS Supervisor) Professor Faculty of Pharmaceutical Sciences Tokyo University of Science 2641 Yamazaki, Noda 278-8510 Japan E-mail: <u>shinaoki@rs.tus.ac.jp</u> Tel No: +81-4-7121-3670
- 4. Dr. Cesar Echeverría (Current Supervisor)

 Faculty of Medicine
 University of Atacama
 Copiapo- 1532502
 Chile
 E-mail: cesar.echeverria@uda.cl
 Mobile No: +56 9 9279 8354

I hereby declare that all the information stated above is true to the best of my knowledge.

J. Hambaby

J. Haribabu





RESEARCH SUMMARY

Cancer is predicted to cause 20 million new cases and 13.1 million deaths in 2030. The research on the anticancer properties of metal complexes gained much importance after the discovery of cisplatin by Rosenberg (1967). The only three globally approved metallodrugs for chemotherapy treatment in the market are platinum-based drugs. However, tumor resistance to platinum drugs is a major problem apart from their deleterious side effects (neurotoxicity, nephrotoxicity, *etc.*,) due to their non-specific activity. Nonetheless, these drugs dominate the cancer world as of now. Therefore, my doctoral thesis work focused on the design and synthesis and characterization of metal complexes bearing heterocyclic thiosemicarbazone (TSC) / thiourea ligands for biological applications. The binding efficacy of the compounds with biomolecules was evaluated using spectroscopic methods. Further, docking technique was employed to understand the binding of the complexes with biomolecular targets. The complexes were also screened for their cytotoxicity against various cancer and normal cell lines, and the results were compared with well-known anticancer agents.

A series of metal [Ni(II) / Zn(II) / Cu(II)] complexes bearing heterocyclic (isatin, indole and 3-acetylcoumarin) based TSCs was synthesized and characterized, out of which some complexes exhibited remarkable cytotoxicity [IC₅₀ < **0.1** μ M (A549 and MCF7)], which was comparable with well-known anticancer drugs. The morphological changes assessed by Hoechst staining revealed that the cell death occurred by apoptosis (*Dalton Trans.* 2020, *Spectrochim. Acta A* 2021, *RSC Adv.* 2015, *J. Biol. Inorg. Chem.* 2018, *J. Inorg. Biochem.* 2018, *Inorg. Chim. Acta* 2016 & 2017, *Polyhedron* 2017, *J. Mol. Struct.* 2015, 2016, *etc.*).

Pd(II) complexes featuring indole/isatin appended TSC ligands showed good cytotoxic activity against A549, MCF7 and HepG-2 cells and the effect of substitution towards DNA and BSA binding ability of the complexes was revealed through molecular docking studies (*Inorg. Chim. Acta* 2017, *New J. Chem.* 2018). Novel Pd(II) complexes containing pyrazole / chromone TSC have been synthesized through Michael addition, ring opening and cyclization. To the best of our knowledge, these are the first report on such type of complex formation and conversion of chromone TSC into pyrazole based thiourea moiety. These Pd(II) complexes displayed potential anticancer activity [IC₅₀ = **0.1-10.4** μ M (PANC-1, HeLa and HepG-2)] and complexes induced apoptosis through mitochondrial signaling pathway and G0/G1 cell cycle arrest in cancer cells (*J. Inorg. Biochem.* 2020 and *Inorg. Chem.* 2020).

Water-soluble mono- and binuclear Ru(II)-arene complexes containing indole based TSC / thiourea / guanidine ligands exhibited significant growth inhibition on A549, MCF7, HepG-2, HEK 293T, PANC-1 and HeLa cells lines with values ranging from < 0.1 to 46.1 μ M in 24 h and complexes are able to induce morphological changes and inhibit the size, number of colonies and induce cell cycle arrest in the sub-G1 phase and apoptosis cell death (*Organometallics* 2018 & 2019, *Dalton Trans.* 2015, *New J. Chem.* 2016, *ChemistrySelect* 2018). Ru(II)-arene complexes as inhibitors of amyloid β (A β) peptide aggregation and A β -induced cytotoxicity (ChemistrySelect 2017). Advantageously, complexes exhibited less toxicity against normal cells. The Ru(II) complexes cleaved the supercoiled DNA without the need of any external agent. Taken together,





Ru(II)-arene complexes possessed potent antitumor activity; it could be a promising lead candidate for the potential treatment of human cancer cell lines.



Figure 1. Outline of my doctoral thesis work.

JSPS Post-Doctoral work: On the other hand, during Postdoctoral Fellowship from Japan Society for the Promotion of Science synthesized green-emitting tris-, bis-, and mono (cationic peptide) hybrids [peptide = KKKGG (K: lysine, G: glycine)] of cyclometalated Ir(III) complexes (IPHs) through multistep reactions for anticancer and biomarkers applications (Figure 2). The tris-IPHs showed potential anticancer activity with an EC50 value of 1.5 μ M against Jurkat (T-lymphocyte leukemia) cancer cells and found that a positive correlation between the number of KKKGG units on the Ir(tpy)₃ core and their anticancer activity. Strong green emission was detected in dead Jurkat cells. Mechanistic studies of cell death suggest that IPHs and celastrol induce paraptotic cell death in Jurkat cells with the vacuolization of the cytoplasm, mitochondria, the ER, and lysosomes, as confirmed by TEM images of Jurkat cells (*Eur. J. Inorg. Chem.*, 2021, 1796-1814). One paper is under review in *Moleculres.*, and one more paper to be submitted to *Inorganic Chemistry*.



Figure 2. Outline of JSPS Post-Doctoral work.

Current Work: Currently, I am researching the design and synthesis of organometallic Ru(II)arene, Ir(III), and Pt(II) complexes with chiral thiourea VEGFR-2 inhibiting ligands for multiple targeting of metastatic cancers and their mechanism of action.





Most important Outcome of my research work as follows:

- Novel synthetic methods for the synthesis of coordination compounds under mild conditions have been reported and the first-time synthesis of Pd complexes *via* Micheal addition and conversion of chromone thiosemicarbazone into pyrazole based thiourea moiety has been reported.
- The water-soluble mono- and binuclear Ru(II)-arene complexes with remarkable cytotoxic activity (better than cisplatin) has been synthesized.
- Development of green emitting Ir(III) peptide complexes with the positive relationship between the number of the peptide unit and their anticancer activity through paraptosis.
- Synthesized organometallic metal complexes with good anticancer activity (<0.1 μ M), which will be further sent for animal model studies.
- Development of Pd complexes with higher binding potential towards SARS-CoV-2 main protease than for chloroquine and hydroxychloroquine.