

Curriculum Vitae

Name : Dr. Mainak Das
Date of Birth : 28th October, 1990
Nationality : Indian
Address : Department of Chemistry,
Jagiellonian University, Gronostajowa 2, 30-387, Kraków, Poland, Europe
E-mail : dasabhramainak@gmail.com
Contact No. : +48 516211819; +91 9875438106

Research

NAWA Ulam Fellow Postdoctoral Researcher	Jagiellonian University, Poland, Europe	April, 2021 - till date
Postdoctoral Research Associate	NISER-Bhubaneswar Odisha, India	2020 - 2021
Ph. D.	NISER-Bhubaneswar Odisha, India	2014 - 2020

Title of the Ph.D. thesis: “*Contracted and Expanded Porphyrin analogues: Syntheses, Conformation, Aromaticity and Coordination Chemistry*”. [Thesis supervisor: Prof. A. Srinivasan, NISER-Bhubaneswar]

Research experience and interest

Doctoral Research

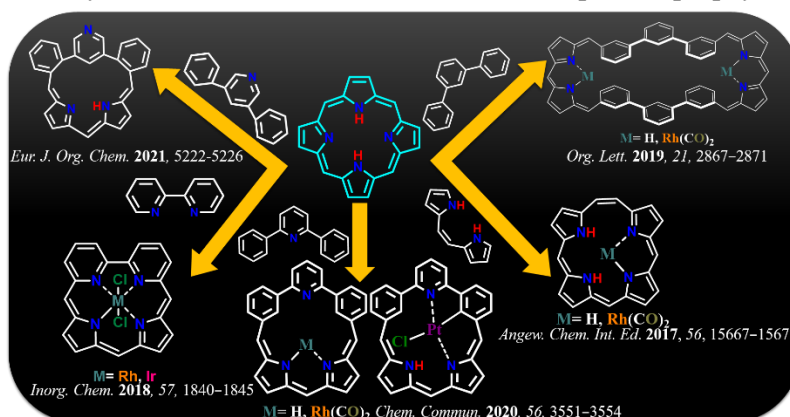
- Design and syntheses of novel contracted and expanded porphyrin derivatives.
- Coordination chemistry of porphyrin analogues and their applications.
- Syntheses of core-modified Calixpyrroles, Calixphyrins and their receptor properties.
- Design and syntheses of novel π -conjugated polycyclic aromatic hydrocarbons (PAH) and exploration of their optoelectronic properties.
- Understanding the structure-reactivity relationship of porphyrinoids.

Postdoctoral Research

- Design and syntheses of water soluble porphyrin derivatives as Diamagnetic Chemical Exchange Saturation Transfer (diaCEST) MRI Contrast agent.
- Design synthetic strategies of double looped macrocycle with strong absorption coefficients in the visible and NIR region.
- Exploration of the aromatic character with potential switching to antiaromatic delocalization using porphyrinoids as a probe.

Research Experience and Achievements during Doctoral degree at NISER, Bhubaneswar:

My research work is mainly focused on syntheses of innovative contracted and expanded porphyrin derivatives and explored their aromatic characteristics, photophysical studies and electrochemical properties. During my doctoral program, I have successfully introduced the arene and pyridine moieties into the macrocyclic framework with miscellaneous bonding mode. These molecules are worthily investigated for the following properties; (i) bipyridyl moiety incorporated monoanionic corrole ring [N₃NH] are exploited to stabilize Rh and Ir in higher oxidation state to tune the luminescence property (*Inorg. Chem.* **2018**, *57*, 1840–1845); (ii) 3,5-diphenylpyridine unit embedded carbatriphyrin embarks hitherto elusive [3.3.1] triphyrin framework (*Eur. J. Org. Chem.* **2021**, 5222–5226); (iii) 2,6-diphenylpyridine unit incorporated isosmaragdyrin with an N₃C₂ core displays intriguing binding mode with Rh^I and Pt^{II} metal ions, where Pt^{II} manifests organo-platinum complex with remarkable metal-arene interaction and form unsymmetrical pincer type of complex inside the macrocyclic core, which is unprecedented in the porphyrin chemistry (*Chem. Commun.* **2020**, *56*, 3551–3554); (iv) Di-(*m-m-m*)terphenyl-embedded oligomeric decaphyrin exhibits an open framework in freebase form and multiple binding pockets stabilizes bis-Rh^I complex (*Org. Lett.* **2019**, *21*, 2867–2871).

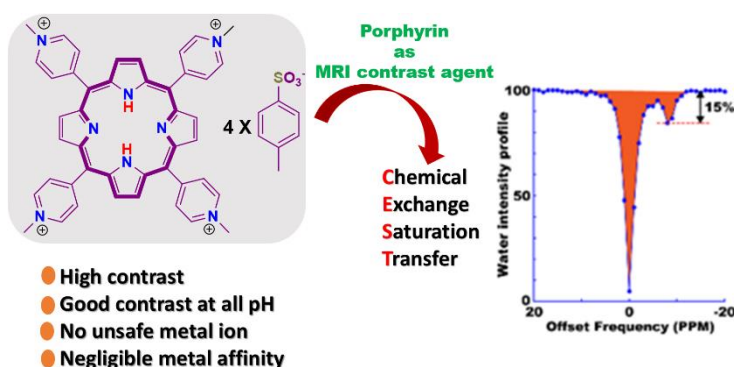


Apart from the antecedent pyri and carbaporphyrins, I also procured *meso*-aryl [20] π homoporphyrin by augmenting one *meso* carbon in the normal porphyrin core. This is the simplest expanded porphyrin with the smallest Möbius topology to date. In this particular project I coined the most dependable synthetic method to obtain bench stable aza-homoporphyrin with the adequate yield in terms of porphyrin chemistry. Furthermore, it binds with Rh^I ion with a unique binding mode and retains the Möbius aromaticity (*Angew. Chem. Int. Ed.* **2017**, *56*, 15667–15671).

In addition, I have also been intensively involved in the synthesis of; (a) *m-o-m* and *p-o-p* terphenyl embedded homocarbaporphyrinoids and their Rh^I complexes, such expanded porphyrin analogues are subjugated to tweak the π conjugation inside the macrocyclic core (*Chem. Eur. J.* **2019**, *25*, 4683 – 4687); (b) bis-4,4'-biphenyl ring embedded octaphyrin with three distinct conformational structures and exploration of their coordination chemistry & aromaticity (*Chem. Eur. J.* **2019**, *25*, 12911 – 12915) [Hot paper]; (c) structurally isomerized bis-biphenyl moieties implanted in hexaphyrin(3.1.1.3.1.1) and octaphyrin(1.1.1.0.1.1.1.0) (*Org. Lett.* **2020**, *22*, 1081–1085) and (d) an unprecedented formation of *meso*-fused β - β' carbaporphyrin dimer and its monomer with keto group. Upon dimerization, the monomeric ligand with dianionic core is transformed into dimeric structure with unique trianionic cores (*Chem. Commun.* **2020**, *56*, 12809 – 12812).

Postdoctoral Research work at NISER, Bhubaneswar:

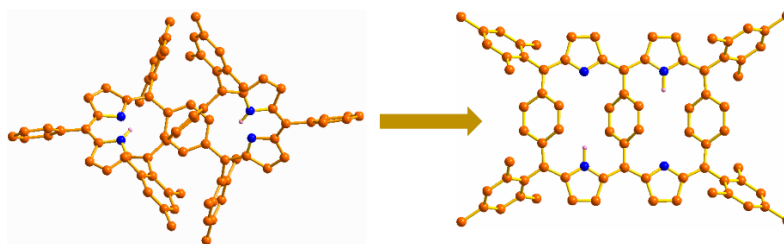
I have synthesized, tetrakis-(N-methyl-4-pyridinium)-porphyrin, a highly water soluble porphyrin derivative which can act as a Diamagnetic Chemical Exchange Saturation Transfer (diaCEST) MRI Contrast agent. The material works proficiently in a physiological condition of pH 7.4 and acidic pH of 6.5 which is quintessential for excretion at 37 °C. This study



would make porphyrin a step closer to be used as a potential diaCEST agent (*New J. Chem.* **2021**, *45*, 1262-1268).

Current research at Jagiellonian University, Poland:

I have synthesized a double looped Hexaphyrin, inspired by expanded porphyrins with split personalities and manifest Hückel-Möbius aromaticity switching. The presence of dual core offers a competitive concomitance of local and global π -conjugation. Also, it is expected to exhibit Baird type of aromaticity at the excited state. (Manuscript under preparation)



Publications

1. **Mainak Das**, B. Adinarayana and A. Srinivasan*, “Recent Advances in the Design and Syntheses of Porphyrinoids by Embedding Higher Analogues of Arene and Pyridine Units”, *ACS Omega* **2021**, *6*, 35204–35212. (Impact Factor: 3.512)
2. **Mainak Das**, Deepak Singh, Sangya Chitranshi, M. Murugavel and A. Srinivasan*, “N-Confused Pyritriphyrin: A New Class of Triphyrin and its Calixphyrin Analogue”, *Eur. J. Org. Chem.* **2021**, 5222-5226. (Impact Factor: 3.021)
3. Subhayan Chakraborty, **Mainak Das**, A. Srinivasan* and Arindam Ghosh*, “Tetrakis-(N-methyl-4-pyridinium)-Porphyrin as a Diamagnetic Chemical Exchange Saturation Transfer (diaCEST) MRI Contrast Agent”, *New J. Chem.* **2021**, *45*, 1262-1268. (Impact Factor: 3.591)
4. M. Murugavel, B. Adinarayana, **Mainak Das**, S. Peruncheralathan, Narasinga Rao Palepu and A. Srinivasan*, “PtCl₂ Mediated Peripheral Transformation of Carbatriphyrin(3.1.1) into *meso*-Fused β - β' Dimer and Its Monomer Analogue”, *Chem. Commun.* **2020**, *56*, 12809 - 12812. (Impact Factor: 6.222)
5. **Mainak Das**, S. Chitranshi, M. Murugavel, B. Adinarayana, C. H. Suresh and A. Srinivasan*, “Isosmaragdyrin with an N₃C₂ core: stabilization of Rh(I) and organo-Pt(II) complexes”, *Chem. Commun.* **2020**, *56*, 3551-3554. (Impact Factor: 6.222)
6. S. Chitranshi[†], **Mainak Das**[†], B. Adinarayana, W.-Y. Cha, D. Kim and A. Srinivasan*, “Structurally Isomerized Bis-Biphenyl Moieties Embedded in Hexaphyrin(3.1.1.3.1.1) and Octaphyrin(1.1.1.0.1.1.1.0)”, *Org. Lett.* **2020**, *22*, 1081-1085. ([†]*equally contributed*). (Impact Factor: 6.005)
7. S. Chitranshi[†], B. Adinarayana[†], **Mainak Das**, W.-Y. Cha, D. Kim and A. Srinivasan*, “Bis-4,4'-biphenyl Ring Embedded Octaphyrin with Three Distinct Conformational Structures”, *Chem. Eur. J.* **2019**, *25*, 12911-12915.[§] ([†]*equally contributed*) ([§]Hot Paper). (Impact Factor: 5.236)
8. **Mainak Das**, B. Adinarayana, M. Murugavel, Subhashree Nayak and A. Srinivasan*, “Di-(*m-m-m*)terphenyl-Embedded Decaphyrin and Its Bis-Rh(I) Complex”, *Org. Lett.* **2019**, *21*, 2867-2871. (Impact Factor: 6.005)

9. B. Adinarayana, **Mainak Das**, C. H. Suresh and A. Srinivasan*, “Homocarbaporphyrinoids: The *m-o-m* and *p-o-p* Terphenyl Embedded Expanded Porphyrin Analogues and Their Rh^I Complexes”, *Chem. Eur. J.* **2019**, 25, 4683-4687. (Impact Factor: 5.236)
10. B. Adinarayana[†], M. Murugavel[†], **Mainak Das**, Narasinga Rao Palepu and A. Srinivasan*, “Rhodium(III) and Iridium(III) Bipyricorrole Complexes: Syntheses, Structures, and Properties”, *Inorg. Chem.* **2018**, 57, 1840-1845. ([†]*equally contributed*). (Impact Factor: 5.165)
11. K. S. Anju[†], **Mainak Das**[†], B. Adinarayana, C. H. Suresh* and A. Srinivasan*, “*meso*-Aryl [20]π Homoporphyrin: The Simplest Expanded Porphyrin with the Smallest Möbius Topology”, *Angew. Chem. Int. Ed.* **2017**, 56, 15667-15671. ([†]*equally contributed*). (Impact Factor: 15.34)

Research Skills

- Experienced in synthesis of **macrocyclic ligands** (e.g. Porphyrin analogues / derivatives) and explore its coordination chemistry in particular stabilization of **organometallic complexes**.
- Experienced in characterizing compounds with various techniques such as **UV-Visible, Fluorescence, NMR, IR, Mass**, Single-crystal X-ray diffraction (**XRD**) and Cyclic voltammetry (**CV**).
- Experienced in handling instruments such as **UV-Vis, IR, Fluorescence, NMR spectroscopy, Mass spectrometry, Cyclic voltammetry (CV)** and **Single-crystal X-ray diffraction**.
- Trained in computer softwares such as **ChemBioDrawUltra 12.0**, MS Windows & Office 2013, Origin 8.5, Endnote X7, **MestReNova, TopSpin 3.6.0, Mercury, Ortep and Diamond**.
- Capable of **solving** and visualizing structures from **single-crystal X-Ray diffraction data** with **Olex system**.

Conferences and Poster Presentations

- “20π Homoporphyrin: The Smallest Expanded Porphyrin with Möbius Topology”, **Mainak Das**, B. Adinarayana, Ch. Sangya and A. Srinivasan* in 5th Symposium on Advanced Biological Inorganic Chemistry (SABIC-2017), January 7-11th, 2017. Jointly organized by the Tata Institute of Fundamental Research (TIFR) and Indian Association for the Cultivation of Science (IACS) at Kolkata. (**Poster Presentation**).
- “Carbahomoporphyrins: Allowed and restricted conjugation in homoporphyrinoids by incorporation of *o*-terphenyl system”, **Mainak Das**, B. Adinarayana and A. Srinivasan* in International Symposium on Modern Trends in Inorganic Chemistry-XVII (MTIC-XVII), December 11-14th, 2017. Jointly organized by Department of Chemistry, Indian Institutes of Science Education and Research (IISER) Pune, National Chemical Laboratory (NCL) Pune and Savitribai Phule Pune University. (**Poster Presentation**).

- “Core-modified Isosmaragdyrin[1.1.1.0.0] and Its Rh(I), organo Pt(II) Complexes”, **Mainak Das** in National Bioorganic Chemistry Conference (NBCC-2018), 22nd–24th December 2018, Organized by NISER Bhubaneswar at Bhubaneswar. (**Oral Presentation**).

Career Achievements

- **Received Merit Prize and Scheme of Scholarship for College and University Students** sponsored by Ministry of Human Resource Development (MHRD), Government of India for securing high position in Higher Secondary Examination (+2 level).
- Qualified **National Eligibility Test (NET)** Lectureship in June-2014, conducted by Council of Scientific & Industrial Research (CSIR), Government of India.
- Qualified **Graduate Aptitude Test in Engineering (GATE) examination** in February-2014 and 2015, conducted by Department of Higher Education, Ministry of Human Resource Development (MHRD), Government of India.
- Best poster awardee of **International Symposium on Modern Trends in Inorganic Chemistry-XVII (MTIC-XVII)**, December 11-14th, 2017. Jointly organized by Department of Chemistry, Indian Institutes of Science Education and Research (IISER) Pune, National Chemical Laboratory (NCL) Pune and Savitribai Phule Pune University, India. Award was given by Dalton Transactions (Royal Society of Chemistry).
- **Polish National Agency for Academic Exchange (NAWA) Ulam Fellowship - 2020** for Postdoctoral research in Poland, Europe.

Teaching experience

Teaching assistant for Laboratory based practical courses for first year under graduate students at NISER-Bhubaneswar.

References

Prof. A. Srinivasan,
School of Chemical Sciences,
National Institute of Science Education and
Research (NISER), Bhubaneswar-752050, Odisha,
India. E-mail: srini@niser.ac.in

Dr. Krishnan Venkatasubbaiah,
School of Chemical Sciences,
National Institute of Science Education and
Research (NISER), Bhubaneswar-752050,
Odisha, India. E-mail: krishv@niser.ac.in

Prof. Samaresh Bhattacharya,
Department of Chemistry, Jadavpur University,
188, Raja S.C. Mallick Rd,
Kolkata-700032, West Bengal, India. E-mail:
samaresh_b@hotmail.com

Dr. S. Peruncheralathan,
School of Chemical Sciences,
National Institute of Science Education and
Research (NISER), Bhubaneswar-752050,
Odisha, India. E-mail: peru@niser.ac.in

I hereby declare that the particulars furnished above are complete and correct to the best of my knowledge and belief.

Yours sincerely,
Mainak Das
(Mainak Das)