

# RENJITH THOMAS PhD, FRSC

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Associate Professor & Head, Department of Chemistry  
Director, Centre for Theoretical and Computational Chemistry  
St Berchmans College (Autonomous), Mahatma Gandhi  
University  
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H-Index: 41

## CURRENT ROLES

Head: Dept of Chemistry (2022-)  
Research Supervisor: Mahatma Gandhi University  
Director: Centre for Theoretical and Computational Chemistry (2022-)  
Member: IQAC (2021-)

## RESEARCH INTERESTS

Theoretical solvation science, Machine Learning in Solvation Dynamics  
Theoretical organic chemistry- Chemical bonding, sulphur centered hydrogen bonds, non-covalent interactions  
Structural investigations, Drug design, Machine Learning in Drug Discovery  
Synthesis of medicinally active compounds and drug delivery  
Theoretical modelling of excited state phenomena

## EDUCATION

**PhD**  
**(Theoretical Chemistry)** Bharathidasan University, Tiruchirappalli. Advisor: Dr G Vijayakumar  
Title - *Electronic structure and reactivity of some bioactive imidazole and pyrazole analogues: An incisive theoretical investigation, 2019*

**MSc Chemistry** Gandhigram Rural University. A Grade, First rank with gold medal  
Supervisor: Prof MG Sethuraman, 2002

**BSc Chemistry** St Berchmans College, Mahatma Gandhi University, 2000

## ACADEMIC POSITIONS

<b>Professor*</b>	St Berchmans College (Eligible from 2022)
<b>Associate Professor</b>	St Berchmans College 2019-2022
<b>Assistant Professor Stage-3</b>	St Berchmans College 2015-2019
<b>Assistant Professor Stage-2</b>	St Berchmans College 2010-2015
<b>Assistant Professor Stage-1</b>	St Berchmans College 2004-2010
<b>Lecturer</b>	
<b>Lecturer (Guest)</b>	Bishop Kurialacherry College Amalagiri 2003 –2004
<b>Lecturer (Guest)</b>	KKTM Government College, 2002-2003 (6 months)
<b>*formalities pending</b>	

## EDITORIAL ASSIGNMENTS

<b>Associate Editor</b>	Journal of Computational Biophysics and Chemistry (World Scientific IF 2.2) (2023-)
<b>Editor</b>	BMC Chemistry (Springer Nature group) IF 4.09 (2021-)
<b>Associate Editor</b>	Frontiers in Chemistry, Theoretical and Computational Chemistry Division (2022-) IF 5.22
<b>Guest Associate Editor</b>	Frontiers in Chemistry special issue on drug repurposing (Theoretical and Computational Chemistry) IF 5.2 (2021-22)
<b>Editorial Board Member</b>	Polytechnic Journal
<b>Chief Editor</b>	Academic Reviews (Science), In house journal of St Berchmans College

## PUBLICATIONS

Published- 158	Communicated – 10
H-index- 41	Book Chapters-2 Editor of Books-1 (List attached at the end)

## RECOGNITIONS AND AWARDS

- Visiting Researcher: University of Novi Sad, Serbia using RSC Collaboration Grant (2024 April-May)
- Fr Dr Jose Thekkan All India Award for the Best Teacher, Christ College, Irinjalakuda (March, 2024)
- Visiting Professor: Saveetha University, Chennai, Centre for Molecular Medicine and Diagnostics (2023-)

- Best Author Award, Elsevier Publications and Journal of Indian Chemical Society (2023)
- Prof Sivaprasad Award for the best college teacher in Kerala (2023)
- Listed as the world's top 2% scientists published by Stanford University and Elsevier (2021, 2022 & 2023)
- Wiley Top Cited Article 2021-22 in Applied Organometallic Chemistry (February, 2023)
- Wiley Top Cited Article 2021-22 in Vietnam Journal of Chemistry (February, 2023)
- Elected to Executive Council of Kerala Academy of Sciences (2022-)
- Citation in recognition of outstanding contributions to chemistry teaching and research, SB College Alumni Association (2022)
- Rank # 1 in AD Scientific Index for the top Scientist at St Berchmans College.
- Gold medal from Gandhigram Rural University for getting First Rank in M.Sc Chemistry (2002)
- Young Scientist Program, Government of India (2002) at Tropical Botanical Garden and Research Institute (TBGRI)
- Visiting Teacher Fellow of Indian Academies of Science with Prof KL Sebastian, Indian Institute of Science, Bangalore (2008)

## **RESEARCH GROUP AT CENTRE FOR THEORETICAL AND COMPUTATIONAL CHEMISTRY**

### **Post Doctoral Researchers**

Dr Jisha Mary Thomas (Post Doc) (2022-)

Dr Mekha Susan Rajan (Post Doc) (2022-)

Dr Kavimani G (Post Doc) (2023-)

### **PhD Students**

Rajimon KJ (PhD student) Organic Chemistry & Aspire Fellow

Manjesh Mathew (PhD student) Theoretical Chemistry

Francis Thomas (PhD student) Theoretical Chemistry

Sneha Sunny (PhD student) Theoretical Chemistry

Meera Kattoor, KCSTEC Fellow (PhD student) Theoretical Chemistry

### **Aspire Visiting Fellow (Govt of Kerala)**

Busharamol (PhD student, Physics, MG University) June 2023-

### **Post graduates and Graduates**

Mr Mebin Varghese (MSc Researcher) (2022-)

Sunisha Nair (KTPRI MSc Research Intern) (2022-23)

Sreelakshmi N MSc (2022-23)

Megha Thomas, Angana, Rencemon MSc (2023-24)  
Ananya Prakash (KPTRI MSc Research Intern, 2023-24)  
Navya, Kannur University (KTPRI MSc Research Intern 2023-24)

### Alumni

Dr T Pooventhiran (Post Doc 2019-22), currently at IISER Kolkatta  
Dr N Elangovan (Post Doc) (2021-23)

### Visitors

Ms Athira Maria John, CHRIST, Bangalore (2019)  
Mr Arnav Paul, NISER Bhubaneshwar (2021) (YSL Fellow)  
Ms Prathyusha, IISER Thiruvananthapuram (2022) (YSL Fellow)  
Dr Santhy Mathew St Joseph's College, Bangalore (2022) (Visiting Faculty)  
Mr Tobin Varkey Simpson, St Joseph's College, Bangalore (2022, 2023) (Visiting Faculty)  
Fr Dr Roshan Castellano, Research Director, St Joseph's University, Bangalore (February 2023) (Visiting Faculty)  
Renjith Pillai, University of Alabama, USA (2023-24) (Visiting Student)

### RESEARCH FUNDINGS

1. **RSC Collaboration Grant (2023-24):** Triazatruxene Derivatives for Next-Gen OLEDs: Insights from Quantum Chemistry and Machine Learning  
Collaborative work with Prof Stevan Armakovic, University of Novisad, Serbia
2. **King Abdulaziz University Deanship Combined Project (2022):** Design and synthesis of anticancer Schiff bases (Co Investigator) Under Progress
3. **RSC Research Fund Grant (2021-22):** QM/MM modelling of deexcitation dynamics after photo-excitation in solution of photosensitizers used in photodynamic therapy (Principal Investigator)
4. **King Abdulaziz University Deanship Combined Project (2021-22):** Designing a molecular library of anticancer heterocycles with imidazole and pyrazole backbone using *insilico* tools: Detailed structural profile and dynamics (Co Investigator)
5. **UGC Project (2013-2015)** Title- Computational studies on the substituent effects on cycloaddition reactions.
6. **UGC Project (2006-2008)** Title- Theoretical investigations into the factors affecting rotation about single bonds.

## **PRINCIPAL COLLABORATORS**

- Dr Ralph Puchta, University of Erlangen, Germany
- Prof Miyum Kim, Gancheon University, South Korea
- Dr Stevan Armarkovic, University of Novisad, Germany
- Dr Elham Shafik Aazam, King Abdulaziz University, Saudi Arabia
- Dr Penny Govender, University of Johannesburg, South Africa

## **SCIENTIFIC COMMUNITY ENGAGEMENT: MEMBERSHIP IN PROFESSIONAL BODIES**

1. Fellow, Royal Chemical Society, London (FRSC)
2. Member, American Chemical Society (ACS)
3. Fellow, Indian Chemical Society (FICS)
4. Fellow, Young Academy of India
5. Life member, Indian Society for Atomic and Molecular Physics (ISAMP)
6. Life Fellow, Indian Society for Radiation and Photochemical Sciences (ISRAPS)
7. Member, Chinese Chemical Society
8. Member, Kerala Academy of Sciences
9. Hon member, Kerala Theoretical Physics Research Initiative
10. Member, Kerala Magnetic Resonance Society

## **SCIENTIFIC OUTREACH: REVIEWER**

ACS Applied Nano Materials, J. of Chemical and Engineering Data, International J. of Computational and Theoretical Chemistry, Journal of Molecular Modeling, Spectroscopy Letters, J. of Theoretical and Computational Chemistry, Spectrochimica Acta A: Biomolecular Spectroscopy, Indonesian J. of Chemistry, Chemistry Select, Physical Chemistry Chemical Physics, Powder Technology, Computational Biology and Chemistry, J. of Cluster Science, CrystEngComm, J. of Biomolecular Structure and Dynamics, Korean Bulletin of Chemistry, Chemical Physics Letters, Nature Scientific Reports, In Silico Pharmacology, Journal of Indian Chemical Society, MDPI- Chemistry, MDPI, J. of Molecular Structure, J. of Molecular Liquids, Theoretical Chemistry Accounts, Indian J of Chemistry, Vietnam J. of Chemistry, J. of Indian Chem Society, ACS Applied Energy Materials, J of Physical Chemistry, J of Chemical Physics

## **SCIENTIFIC OUTREACH: INVITED TALKS**

1. Invited Talk, Faculty of Science, University of Novi Sad, Serbia, April 2024

- (Scheduled)
2. Invited Talk, Faculty of Science, University of Kragujevac, Serbia, April 2024 (Scheduled)
  3. Invited Talk, FDP, SRM University, Chennai, February 14, 2024 (Scheduled)
  4. Invited Talk, St Joseph's University, Bangalore, November, 2023
  5. Invited Talk, National Conference, AVS College, Villupuram, Tamil Nadu, October, 2023
  6. Invited Talk, National Science Day Celebrations of Kerala Academy of Sciences at BAM College, February 28, 2023
  7. Invited Talk, DFT Workshop, St Dominic's College, February 17, 2023
  8. Invited Talk, Mannar College, Madurai, January 12, 2023
  9. Invited Talk, Nadar Mahajana Sangam S V Nadar College, Madurai, 17, November, 2022
  10. Invited Talk, Assumption College, Changanassery, October, 2022
  11. Keynote Speaker, Vivekananda College for Women, Trichenkode, Erode May 2022
  12. Invited Talk, Faculty Development Programme, St Joseph's College for Women, Alappuzha, January 2022
  13. Invited Talk, International Conference on Materials Science and Applied Physics, Mizoram University, November, 2021
  14. Invited Talk. International Conference on Materials Science, Turkey, October, 2021
  15. Invited Talk, National Webinar, American College, Madurai, June 2021
  16. Invited Talk, Shri Shivaji Science College, Amravati, Maharashtra, April 2021
  17. Invited talk, Muthiyammal College of Arts and Science, Tamil Nadu, April 2021
  18. Invited Talk, St Joseph's College, Allapuzha, February 2020
  19. Invited Talk, National Seminar, Adikavi Nannaya University, Andra Pradesh, May 2020
  20. Invited Talk, National Seminar, SN College, Chathannur, November 2017
  21. Invited Talk, Thermodynamics of Biological Systems- MACFAST College, Thiruvilla, September, 2014
  22. Invited Talk, Chemistry in the context of Science and Religion- B.K Institute for Science and Religion November 2006

## **SCIENTIFIC OUTREACH: CONFERENCE PRESENTATIONS**

1. Oral Presentation Two-day National Seminar on Materials for a Sustainable Future, St. Paul's College Kalamassery in association with College Department Council, MG University on 12<sup>th</sup> and 13<sup>th</sup> October 2023. (Rajimon KJ)
2. Oral Presentation DST-SERB and CSIR Sponsored International Conference on New Materials for Industry and Medicine (NMIM'24) organised by, PSGR Krishnammal College for Women on 30<sup>th</sup> and 31<sup>st</sup> January 2024. Best paper Award (Rajimon KJ)

3. International Seminar on Advances of Nano Materials in Sensing, Energy and Biomedical Applications organised by KSCSTE, BCM College Kottayam on 8<sup>th</sup> and 9<sup>th</sup> February 2024. (Rajimon KJ)
4. Oral Presentation, National Conference on Contemporary Topics in Chemistry, February, 2023 (Mebin Varghese, Second best oral presentation award)
5. Oral Presentation, National Conference, Calicut University, February, 2023 (Rajimon KJ)
6. Oral Presentation, Kerala state Conference, Fatima Mata National College, February, 2023 (Rajimon KJ)
7. Poster Presentation, RSC-PCCP & IISER Desktop conference, May 2021 (Renjith Thomas)
8. Poster Presentation, RSC-PCCP & IISER Desktop conference, May 2021 (Arnav Paul)
9. Oral Presentation, National Conference on Analytical and Materials Chemistry for Everyday Life, February 2021 (Dr T Pooventhiran, Best presentation award)
10. Oral Presentation, India International Science Foundation, November 2020 (Utsab Bhattacharya)
11. Oral Presentation, India International Science Foundation, November 2020 (Arnav Paul)
12. Poster Presentation, International Conference on Supramolecular and Photochemistry, January 2020 (Renjith Thomas)
13. Presentation, Virtual Conference on Computational Chemistry, August 2019 (Athira M John)
14. Poster Presentation, International Conference on Functional Materials St Berchmans College, Changanassery, September 2018 (Renjith Thomas)
15. Poster Presentation, National Seminar on Recent Advances in Chemical Science (RACS 2017), University College, Trivandrum, March 13 & 14, 2017 - Paper Presentation. (Renjith Thomas)
16. Poster Presentation, National Seminar on Supramolecular and Nanochemistry, Assumption College, Changanaserry, November 16 & 17, 2017 - Paper Presentation. (Renjith Thomas)
17. Oral presentation, National Seminar on Advances in Natural Products Chemistry – Thiruchirapalli- February 2002 (Renjith Thomas)
18. Linus Pauling Lecture in Advanced Quantum Mechanics- Bishop Kurialcherry College May 2006 (Renjith Thomas)

#### **SCIENTIFIC OUTREACH: EVENTS ORGANISED**

1. Chairman, National Conference on Contemporary Topics in Chemistry, St Berchmans College, February, 2023
2. Chairman, National Science Day celebrations of Kerala Academy of Sciences at St Berchmans College, February 28, 2023
3. Organiser, National Science Day celebrations of Kerala Academy of Sciences at BAM College, February 28, 2023

4. Coordinator, Alumni Lecture Series, Dept of Chemistry, St Berchmans College, 2020
5. Advisory Board, Progress and Promises in Chemical Sciences, CHRIST, Bangalore, 2019
6. Advisory Board, International Conference on Advanced Nanomaterials for Energy, Engineering, Medical and Biological Applications, 15-18 December 2019
7. Committee member: International Conference of Functional Materials: Venue: St Berchmans College 11, 12 December 2018
8. Organizing Secretary: UGC sponsored First Indian National Seminar on Emerging Trends in Chemoinformatics: Venue: St Berchmans College 7,8,9 March 2006

## **OTHER CERTIFICATIONS**

Certificate of training in quality control, testing and analysis of Rubber Products, Ministry of Industry, Government of India (2000)

Passed National Eligibility Test (JRF-NET) of UGC /CSIR (2002)

Passed Graduate Aptitude Test in Engineering (GATE) (2003)

Certificate in MS Office Gandhigram Rural University (2002)

NPTEL course (2018) : Atomic structure and chemical Bonding offered by Indian Institute of Technology- Madras.

## **PERSONAL DETAILS**

Fathers name : K. J. Thomas (Late)  
Sex : Male  
Date of Birth : 24, February 1980.  
Marital status : Married to Dr Anila Skariah, 3 kids  
Nationality : Indian  
Languages known: English, Malayalam (mother tongue)

## **MAJOR POISTIONS HELD IN COLLEGE**

Director: Department of Short-Term Programs, St Berchmans College (2021-22)

Director: Centre for Interdisciplinary Research, St Berchmans College (2021-22)

Secretary and elected member: Staff Council (2014-17)

Member and Criteria Head: IQAC (2021-)

Elected Member: Cooperative Society (2010-2013)

## **BOOKS/CHAPTERS**

1. Photosensitizers and Applications (Edited by Davor Margetic and Renjith Thomas), Nova Publishers 2021



2. Chapter: Renjith Thomas, T Pooventhiran, Comprehensive quantum mechanical study of structural features, reactivity, molecular properties and wave function based characteristics of Capmatinib, (Ed Dibya R Pai) Advanced Materials and Nano systems: Theory and Experiment, Bentham Publishers, 2021
3. Chapter: Renjith Thomas, Anila Skariah Sars Covid-2 : Vaccines, drug repurposing, global health security and mental well-being, (Ed Dhiraj Singh) Covid-10 Crisis and India, New Delhi June 2021

## RESEARCH PAPERS (R. Thomas) H Index 41

Please see the following link for the updated list

[https://scholar.google.co.in/citations?hl=en&user=3Vj0QjsAAAAJ&view\\_op=list\\_works&sort\\_by=pubdate](https://scholar.google.co.in/citations?hl=en&user=3Vj0QjsAAAAJ&view_op=list_works&sort_by=pubdate)

**Total number 158**

- [1] E.S. Aazam, R. Thomas, Solution stage fluorescence and anticancer properties of azomethine compounds from sulpha drugs: Synthesis, experimental and theoretical insights, *J. Mol. Struct.* 1295 (2024) 136669.
- [2] J. S. Al-Otaibi, Y.S. Mary, Y.S. Mary, R. Trivedi, B. Chakraborty, R. Thomas, Cluster formation between an oxadiazole derivative with metal nanoclusters (Ag/Au/Cu), graphene quantum dot sheets, SERS studies, and solvent effects, *Struct. Chem.* 34 (2023) 867–877.
- [3] S. Tabassum, P. Thangaiyan, S. Govindaraju, N.K. Daniel, R. Thomas, Pyrazole Derivative Containing Naphthalene Moiety: Cytotoxicity (Breast and Cervical Cancer), Antibacterial and Antifungal Studies Using Experimental and Theoretical Tools, *Polycycl. Aromat. Compd.* 43 (2023) 8544–8561.
- [4] A. Kanagavalli, G. Thilagavathi, R. Jayachitra, N. Elangovan, S. Sowrirajan, K.R. Shadakshara Murthy, R. Thomas, Synthesis, electronic structure, UV--vis, wave function, and molecular docking studies of Schiff base (Z)-N-(Thiazol-2-yl)-4-((Thiophene-2-ylmethylene) Amino) Benzenesulfonamide, *Polycycl. Aromat. Compd.* 43 (2023) 8710–8728.
- [5] M.A. Bakht, A.I. Alharthi, P. Thangaiyan, A. Ahmad, I. Ali, R. Thomas, Interaction of serotonin and histamine with water and ethanol: Evidence from theoretical investigations, *Comput. Theor. Chem.* 1228 (2023) 114299.
- [6] R.A. Kumar, S.J. Al-Otaibi, Y.S. Mary, Y.S. Mary, N. Acharjee, R. Thomas, R.R. Pillai, T.L. Leena, Surface adsorption of adenine on pristine and B/N/O/P-doped coronene as biosensing substrate for DNA detection-DFT Study, *J. Mol. Liq.* (2023) 123546.
- [7] E.S. Aazam, R. Thomas, Understanding the behavior of a potential anticancer lamotrigine in explicit solvent (water and DMSO) using quantum mechanical tools and abinitio molecular dynamics, *Chem. Phys. Impact.* (2023) 100404.
- [8] A.B. Abraham, A.Y. Alzahrani, R. Thomas, Exploring non-covalent interactions between caffeine and ascorbic acid: their significance in the physical chemistry of drug efficacy,

- Zeitschrift Für Phys. Chemie. (2023).
- [9] J.S. Al-Otaibi, Y. Sheena Mary, Y. Shyma Mary, R. Thomas, Electronic Structure, Solvation Effects and Wave Function Based Properties of a New Triazole Based Symmetric Chromene Derivative of Apigenin, *Polycycl. Aromat. Compd.* 43 (2023) 2810–2822. <https://doi.org/10.1080/10406638.2022.2055583>.
- [10] P. Surendar, T. Pooventhiran, S. Rajam, D.J. Rao, N. Manigandan, A. Irfan, R. Thomas, Organic Quasi-Liquid Schiff Bases from Biomolecules: Synthesis, Structure and Quantum Mechanical Studies, *Biointerface Res. Appl. Chem.* 13 (2023) 1–46.
- [11] T. Pooventhiran, K.R.S. Murthy, R.K. Joseph, R. Thomas, Study of the Electronic Properties of a Fluoropyrazolecarbonitrile Derivative and Enhancement of Spectral Properties on Adsorption with Fullerene, *Biointerface Res. Appl. Chem.* 13 (2023). <https://doi.org/10.33263/BRIAC134.342>.
- [12] T. Pooventhiran, A.Y.A. Alzahrani, K.J. Rajimon, R. Thomas, Solvent interaction and dynamics of neurotransmitters L-aspartic acid and L-glutamic acid with water and ethanol, *J. Mol. Struct.* 1273 (2023). <https://doi.org/10.1016/j.molstruc.2022.134347>.
- [13] A. Kanagavalli, R. Jayachitra, G. Thilagavathi, M. Padmavathy, N. Elangovan, S. Sowrirajan, R. Thomas, Synthesis, structural, spectral, computational, docking and biological activities of Schiff base (E)-4-bromo-2-hydroxybenzylidene) amino)-N-(pyrimidin-2-yl) benzenesulfonamide from 5-bromosalicylaldehyde and sulfadiazine, *J. Indian Chem. Soc.* 100 (2023). <https://doi.org/10.1016/j.jics.2022.100823>.
- [14] R. Jayachitra, G. Thilagavathi, A. Kanagavalli, N. Elangovan, A. Sirajunnisa, S. Sowrirajan, R. Thomas, Synthesis, Computational, Electronic spectra, and molecular docking studies of 4-((diphenylmethylene)amino)-N-(pyrimidin-2-yl)benzenesulfonamide, *J. Indian Chem. Soc.* 100 (2023). <https://doi.org/10.1016/j.jics.2022.100836>.
- [15] G. Thilagavathi, R. Jayachitra, A. Kanagavalli, E. N. A. Sirajunnisa, S. S, R. Thomas, Synthesis, computational, molecular docking studies and photophysical properties of (Z)-N-(pyrimidin-2-yl)-4-(thiophen-2-ylmethylene)amino) benzenesulfonamide, *J. Indian Chem. Soc.* 100 (2023). <https://doi.org/10.1016/j.jics.2022.100835>.
- [16] K.J. Rajimon, N. Elangovan, A. Amir, R. Thomas, Schiff bases from chlorine substituted anilines and salicylaldehyde : Synthesis , characterization , fluorescence , thermal features , biological studies and electronic structure investigations, *J. Mol. Liq.* 370 (2023) 121055. <https://doi.org/10.1016/j.molliq.2022.121055>.
- [17] R. Jayachitra, M. Padmavathy, A. Kanagavalli, G. Thilagavathi, N. Elangovan, S. Sowrirajan, R. Thomas, Synthesis, computational, experimental antimicrobial activities and theoretical molecular docking studies of (E)-4-((4-hydroxy-3-methoxy-5-nitrobenzylidene) amino)-N-(thiazole-2-yl) benzenesulfonamide, *J. Indian Chem. Soc.* 100 (2023). <https://doi.org/10.1016/j.jics.2022.100824>.
- [18] T. Sanakarganesan, N. Elangovan, S. Chandrasekar, E. Ganesan, V. Balachandran, S. Sowrirajan, K. Balasubramani, R. Thomas, Synthesis, Hirshfeld surface analysis, computational, wave function properties, anticancer and cytotoxicity activity of di[(p-chlorobenzyl) (dibromo)] (4,7-dimethyl-1,10-phenanthroline)tin (IV) complex, *Inorganica Chim. Acta.* 547 (2023). <https://doi.org/10.1016/j.ica.2022.121361>.
- [19] A. Kanagavalli, R. Jayachitra, G. Thilagavathi, N. Elangovan, S. Sowrirajan, R. Thomas, Synthesis, characterization, computational, excited state properties, wave function, and

- molecular docking studies of (E)-4-((2-hydroxybenzylidene)amino)N-(thiazol-2-yl) benzenesulfonamide, *J. Indian Chem. Soc.* 100 (2023).  
<https://doi.org/10.1016/j.jics.2023.100885>.
- [20] G. Thilagavathi, R. Jayachitra, A. Kanagavalli, N. Elangovan, A. Sirajunnisa, K.J. Rajimon, S. Sowrirajan, R. Thomas, (E)-4-((4-chlorobenzylidene)amino)-N-(thiazole-2-yl) benzenesulfonamide: Synthesis, characterization and electronic structure theory and docking studies, *J. Indian Chem. Soc.* 100 (2023).  
<https://doi.org/10.1016/j.jics.2023.100910>.
- [21] M.A.A.-H. Badawi, A.A. Khairbek, R. Thomas, Computational studies of the CuAAC reaction mechanism with diimine and phosphorus ligands for the synthesis of 1, 4-disubstituted 1, 2, 3-triazoles, *New J. Chem.* 47 (2023) 3683–3691.
- [22] J. Geethapriya, A.R. Devaraj, K. Gayathri, R. Swadhi, N. Elangovan, S. Manivel, S. Sowrirajan, R. Thomas, Solid state synthesis of a fluorescent Schiff base (E)-1-(perfluorophenyl)-N-(o-toly) methanimine followed by computational, quantum mechanical and molecular docking studies, *Results Chem.* 5 (2023) 100819.
- [23] M.A. Bakht, T. Pooventhiran, R. Thomas, M. Kamal, I.U. Din, N.U. Rehman, I. Ali, N. Ajmal, M.J. Ahsan, Synthesis and Biological Evaluation of Octahydroquinazolinones as Phospholipase A2, and Protease Inhibitors: Experimental and Theoretical Exploration, *Molecules.* 28 (2023) 1944.
- [24] J.S. Al-Otaibi, Y.S. Mary, Y.S. Mary, R. Thomas, R.A. Costa, DFT Investigations on the Interactions Between Pyrimidine Derivatives and Ag/Au/Cu Metal Clusters: Solvation Effects and Reactivity Analysis, *J. Clust. Sci.* (2023) 1–12.
- [25] N. Elangovan, T.S. Ganesan, B. Rajeswari, A. Kanagavalli, S. Kokilavani, S. Sowrirajan, S. Chandrasekar, R. Thomas, Solid-state Synthesis, electronic Structure Studies, Solvent Interaction through Hydrogen Bonding, and Molecular Docking Studies of 2,2'-((1,2-Phenylenebis(Azaneylylidene))Bis (Methaneylylidene))Diphenol from o-Phenylenediamine and Salicylaldehyde, *Polycycl. Aromat. Compd.* (2023).  
<https://doi.org/10.1080/10406638.2023.2198723>.
- [26] N. Elangovan, S. Sowrirajan, A.Y.A. Alzahrani, D.S. Rajendran Nair, R. Thomas, Fluorescent Azomethine by the Condensation of Sulfadiazine and 4-Chlorobenzaldehyde in Solution: Synthesis, Characterization, Solvent Interactions, Electronic Structure, and Biological Activity Prediction, *Polycycl. Aromat. Compd.* (2023).  
<https://doi.org/10.1080/10406638.2023.2216833>.
- [27] M.A. Al-Hakim Badawi, M.I. Al-Zaben, R. Thomas, DFT Studies on Mechanism of Organocatalytic Metal-Free Click 32CA Reaction for Synthesis of NH-1,2,3-triazoles, *Catal. Letters.* (2023). <https://doi.org/10.1007/s10562-023-04374-3>.
- [28] J.M. Thomas, R. Thomas, Study of Non-Covalent Interactions Present in the Tapinarof-Ethanol System with Special Emphasis on Hydrogen-Bonding Interactions, *J. Phys. Chem. B.* 127 (2023) 5933–5940. <https://doi.org/10.1021/acs.jpcc.3c03152>.
- [29] J.S. Al-Otaibi, Y.S. Mary, Y.S. Mary, R. Thomas, Evidences of noncovalent interactions between indole and dichloromethane under different solvent conditions, *J. Mol. Model.* 29 (2023). <https://doi.org/10.1007/s00894-023-05623-3>.
- [30] E.P. Diya, M. Unni, K.J. Rajimon, N. Elangovan, K.R.S. Murthy, R. Thomas, Synthesis, spectral features, electronic structure studies, and molecular docking analysis of a

- Schiffbase (E)-1-(4-chlorophenyl)-N-(nitrophenyl)methanimine from 4-chloroaniline and 2-nitrobenzaldehyde, Vietnam J. Chem. (2023). <https://doi.org/10.1002/vjch.202300001>.
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