**B. M. S. COLLEGE OF ENGINEERING, BANGALORE-19**

(Autonomous institute, Affiliated to VTU)

**DEPARTMENT OF CHEMISTRY**

**The activity report of the year 2021**

1. **15th January 2021:** Dr. C. Sampath, Assistant Professor, Published a research paper titled "Design and synthesis of novel 1,3,2- benzoxazaphosphinine-2-one derivatives: an in vitro biological evaluation and in silico approaches" Published by Journal of Taylor & Francis.
2. **19th January 2021:** Dr. M S Dharmaprakash, Professor, Dr. K L Nagashree, Assistant Professor and Dr. S Manjunatha, Assistant Professor, published a research paper titled "Electrocatalytic detection of nitrite at $NiCo_2O_4$ nanotapes synthesized via microwave-hydrothermal method" Published by Journal of Electroanalytical Chemistry.
3. **February 1, 2021:** Dr.Srinidhi R, Faculty, Department of Chemistry presented research paper titled "Gas sensing properties of nanocrystalline nickel ferrite ($NiFe_2O_4$ ) thin films prepared via microwave-assisted process" in the International Conference on Nanoscience and Nanotechnology, (ICONN 2021) organized by Department of Physics and Nanotechnology, SRM IST, India in association with Shizuoka University, Japan; National Chiao Tung University, Taiwan; GNS, New Zealand; University of Rome Tor Vergata, Italy; RMIT University, Australia; Tata Institute of Fundamental Research, India; The Asian Consortium on Computational Materials Science (ACCMS); Indian Physics Association (IPA); Material Research Society of India (MRSI), Indian Carbon Society, Council of Scientific & Industrial Research (CSIR), Indian Science Congress Association (ISCA), Department of Science & Technology (DST) and Springer Nature from February 1-3, 2021
4. **1st March 2021:** New Engineering Chemistry Lab Inaugurated by Sri. Aviram Sharma Trustee, BMSET, Dr. B V Ravishankar Principal, Dr. S Muralidhara Vice Principal, BMSCE.

5. **4th March 2021:** Dr. Srinidhi R, published a research paper titled "Carbonaceous ZnO nanocomposite for sensing of $H_2S$ at sub-ppm concentrations" in the journal of Fullerenes, Nanotubes and Carbon Nanostructures.
6. **26th March 2021:** Dr. C Sampath along with other inventors published an Indian Patent with application number 202141008390 titled "In silico screening of novel sulfonamides as potential antimicrobial drugs docked with protein targets: PDB: 2VF5, 1KZN and 1JIJ and their synthesis using green approach".
7. **29th March 2021:** Dr. Sampath C published a research article titled "Synthesis of novel alkylphosphonates as promising antimicrobial drugs: Computational molecular docking studies" in the journal Phosphorus, Sulfur, and Silicon and the Related Elements, a web of science indexed journal.
8. **30th March 2021:** Dr. Srinidhi R., Dr. S. Manjunatha and Dr. Malini S. have been recognized as a research supervisor in the Department of chemistry from VTU.
9. **31st March 2021:** Dr. Kalyan Raj, published a research paper titled "Multi-applications of new trinuclear Zr-SMI complex" in the Journal of Molecular Structure.
10. **9th - 10th April 2021:** Dr Kirti Agarwal, Professor, Department of Chemistry presented a paper in the International Conference on Energy and Environment (ICEE-2021-Virtual Conference), Title of the paper "Preserve Mountains And Hills To Preserve The Fragile Ecosystem" organized by Jyothi Engineering College, Thrissur, Kerala, India, in association with Indian Society for Technical Education (ISTE)
11. **1st - 5th June 2021:** Dr Srinidhi Raghavan M, Faculty, Department of Chemistry, participated & completed successfully AICTE Training And Learning (ATAL) Academy Online Elementary FDP on "Recent Advances and Challenges in Nanoscale Devices: Design, Materials, and Applications Perspective" at National Institute of Technology Hamirpur.

12. **07th – 09th June 2021:** Dr. C Sampath and Dr. Supriya S, Faculty, Department of CHEMISTRY, Participated in three days FDP program on 'Emerging trends in Pharmaceutical Science' organized by Krishna Teja Pharmacy College, Tirupati, Andhra Pradesh, India
13. **11th June 2021:** Dr Srinidhi Raghavan.M, Faculty, Department of Chemistry, was invited to deliver talks on "Nanoscience – A Tiny Technology" by Dept. of Chemistry, Jindal College for Women, Jindal Nagar, Bengaluru.
14. **11th June 2021:** Dr C Sampath, Faculty, Department of Chemistry, Patent published Title of the invention: Novel synthesis and DFT calculations of 3-phenyl-2-(1H-tetrazol-5-yl) acrylamides under catalyst-free, one-pot cascade reaction Application number: 202141023459
15. **15th June 2021:** Dr C Sampath, Faculty, Department of Chemistry, Patent filed Title of the invention: Computer-aided drug design and green synthesis of novel pyrazole analogues as potential SARS-CoV-2 main protease inhibitors against anti-COVID-19 protein targets
16. **21st June 2021:** Dr M S Dharmaprakash Faculty, Department of Chemistry with Dr. A. Usha Faculty, Department of EEE, patent published titled "Smart Sensor for Biological Real Time Applications Based on Conducting Polymers and Gold Nano Particulates." Application number-2859/CHE/2012
17. **21st – 25th June 2021:** Dr. C Sampath, Faculty, Department of Chemistry, Participated in five days FDP program on ''Green and Sustainable Technologies-Advanced Analytical Techniques 2021 (GST-AAT 2021)' organized by REVA University, Bengaluru, Karnataka, India.
18. **21st– 25th June 2021:** Dr. S Supriya, Faculty, Department of Chemistry, Participated in five days FDP program on ''Insight into Analytical techniques and its applications (IATA - 2021)" organized by Acharya Institute of Graduate Studies
19. **30th June 2021:** Dr. C Sampath, Faculty, Department of Chemistry, Delivered an invited talk in the National Webinar entitled 'In silico evaluation and synthesis of novel sulfonamides as promising anti-viral drugs docked against anti-COVID-19 protein targets' organized by Department of Chemistry (PG), Andhra Loyola College, Vijayawada, Andhra Pradesh, India.
20. **July 2, 2021:** Dr C Sampath, Faculty, Department of Chemistry, Patent published title of the invention: Computer-aided drug design and green synthesis of novel pyrazole

analogues as potential SARS-CoV-2 main protease inhibitors against anti-COVID-19 protein targets, Application number: 202141026750

21. **July 3, 2021:** Dr. M S Dharmaprakash and Dr. S Manjunatha, Faculty, Department of Chemistry, published a research paper titled “Biological activity of PdNPs derived from hemicellulose via microwave assisted green synthesis” in the journal of Current Research in Green and Sustainable Chemistry
22. **July 5, 2021**: Dr. Srinidhi R, Faculty, Department of Chemistry, participated & completed successfully AICTE Training And Learning (ATAL) Academy Online Elementary FDP on "Novel Materials" from 05.07.2021 to 09.07.2021 at Indian Institute of Technology Bhilai
23. **July 10, 2021**: Dr. Supriya S, Faculty, Department of Chemistry, published a research paper titled “An investigation on temperature dependent surface properties of porous carbon nanoparticles derived from biomass". Journal of Nanostructure in Chemistry, Impact factor: 6.391
24. **July 12, 2021**: Dr. Supriya S, Faculty, Department of Chemistry, attended a Seminar conducted by IUCEE Foundations, Topic: “Writing research papers on the Scholarship of Teaching and Learning”
25. **July 13, 2021**: Dr. Supriya S, Faculty, Department of Chemistry, published a Book Chapter Title: Third-Order Nonlinear Optical Application of Organometallic Compounds, Publishers: Nova Science Publishers, Inc.
26. **July 29, 2021:** Dr. G. S. Ananthnag, Faculty, Department of Chemistry delivered an invited talk on “NMR Spectroscopy – Basics and Modern Applications” at Poornaprajna Institute of Scientific Research - Bidalur, Devanahalli, Bengaluru.
27. **July 31, 2021:** Dr. Kirti Agarwal, Faculty, Department of Chemistry was retired from the service. Felicitation farewell function was organized by Department of Chemistry and Institutional level

28. **August 13, 2021**: Dr. Kalyan Raj, Professor & HOD, Department of Chemistry, supervised Mr. N. Suresha (1BM13PGN04) for a Ph.D. pre-submission colloquium with

the thesis entitled "Catalyzed Oxidation Kinetics of Some Drug Molecules: A Mechanistic Investigation"

29. **August 20, 2021:** Dr. C. Sampath, Faculty, Department of Chemistry, filed and published an Indian patent with the title of the invention: Computer-aided molecular docking, physicochemical and ADMET properties of novel bromopyrimidine analogues as potential anti-cancer agents. Application number: 202141036136
30. **August 23, 2021**: Dr. S. Manjunatha, Faculty, Department of Chemistry, participated and completed successfully AICTE Training and Learning (ATAL) Academy Online Elementary FDP entitled "Advances in Waste Treatment Technologies" from 23/08/2021 to 27/08/2021 at Government Engineering College, Modasa, Gujarat, India
31. **August 24, 2021**: Dr. Kalyan Raj and Dr. K. L. Nagashree, Faculty, Department of Chemistry, published a research article titled "Cobalt metal-organic framework for low concentration detection of glucose" in Inorganic and Nano-Metal Chemistry. Web of Science indexed Q3 ranked journal with impact factor: 1.716. https://www.tandfonline.com/doi/full/10.1080/24701556.2021.1966451
32. **August 27, 2021:** Dr. C. Sampath, Faculty, Department of Chemistry, filed and published an Indian patent with the title of the invention: In silico, ADMET properties and anti-viral activity of sesquiterpene lactone analogues against SARS-CoV-2 main protease inhibitors and Indian mutant. Application number: 202111035006
33. **August 31, 2021:** Dr. C. Sampath, Faculty, Department of Chemistry, published a research article titled "Synthesis, $\alpha$-amylase and $\alpha$-glucosidase inhibition and molecular docking studies of indazole derivatives" in the Journal of Biomolecular Structure and Dynamics. Web of Science indexed Q2 ranked journal with impact factor: 3.310. https://doi.org/10.1080/07391102.2021.1947892
34. **September 1, 2021**: Dr. C. Sampath, Faculty, Department of Chemistry, published a research article titled 'Molecular docking of phenolic compounds and Screening of Antioxidant and Anti-diabetic potential of Olea europaea L. Ethanolic leaves extract'. *Arab. J. Chem.*, Elsevier, 2021, 14, 103422. Web of Science indexed Q2 ranked journal with impact factor: 5.16. https://doi.org/10.1016/j.arabjc.2021.103422
35. **September 20$^{th}$ -24$^{th}$, 2021**: Dr. C. Sampath, Faculty, Department of Chemistry, participated in the five-day Faculty Development Programme on 'Advances and challenges in Chemical Science', organized by the School of Sciences (Chemistry), National Institute of Technology (NIT), Andhra Pradesh held from 20$^{th}$-24$^{th}$ September, 2021

36. **September 29th, 2021**: Dr. C. Sampath, Faculty, Department of Chemistry, got an Australian grant patent with the title of the invention: *In silico* screening, physicochemical and pharmacokinetic analysis of novel sulfonamides as potential antimicrobial drugs docked with protein targets: PDB: 2VF5, 1KZN, and 1JIJ. Patent number: 2021105099
37. **October 21, 2021**: Dr. Supriya S, Faculty, Department of Chemistry, published a research article titled "Porous carbon nanoparticles dispersed nematic liquid crystal: influence of the particle size on electro-optical and dielectric parameters" in the journal Liquid Crystals Impact factor: 3.51.
38. **November 2, 2021**: Dr. Kalyan Raj and Dr. Malini S, Faculty, Department of Chemistry, published a research article titled "Donepezil oxidation: complementary chemical and spectroscopic exploration of products, mechanism and kinetics" in the journal of Chemical Papers, DOI: https://doi.org/10.1007/s11696-021-01934-y
39. **November 5, 2021**: Dr. Supriya S, Faculty, Department of Chemistry, published an article titled, "Porous carbons derived from Arecanut seeds by direct pyrolysis for efficient $CO_2$ capture" in the journal "Emergent Materials" in the journal of Emergent mater
40. **November 15-16, 2021**: Dr. Supriya S, Faculty, Department of Chemistry, Attended a two days workshop on "Implementation of NEP 2020" organised by B.M.S College of Engineering in association with VTU
41. **November 15-19, 2021**: Dr. Supriya S, Faculty, Department of Chemistry, Attended 5 days FDP organised by Don Bosco Institute of Technology on "Recent trends in Green Chemistry-2021 (RTGC)
42. **November 20, 2021**: Ms. Arathi K, research scholar Department of Chemistry, online Open Seminar-1 is scheduled on 20th November 2021 (Saturday) at 11.00 AM. The details are as follows: Topic: Studies on the synthesis and Development of Metal Oxide and sulfides for corrosion resistance, Electrodeposition and Photocatalytic Applications, Platform: Google meet link: https://meet.google.com/cfh-xyht-qwh
43. **December 20, 2021**: Dr. Kalyan Raj, Faculty, Department of Chemistry, published a research article titled "Evaluation of Electrochemical and Anticorrosion Properties of Polyaniline-Fly Ash Nanocomposite" in the Hindawi International Journal of Corrosion Volume 2021, Article ID 1547384, 10 pages, DOI: https://doi.org/10.1155/2021/1547384