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DEPARTMENT OF AND HUMANITIES AND SCIENCE JOURNAL PUBLICATIONS AY 2022 – 23

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1	Dr. P. Pandi	Fabrication of self charging supercapacitor based on two dimensional bismuthene-graphitic carbon nitride nanocomposite powered by dye sensitized solar cells	JOURNAL OF ENERGY STORAGE	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57209453416
2	Dr. P. Anthoniammal	Biogenic synthesis of gold nanoparticles using bael fruit juice and its efficacy against human A-549 lung cancer cell line	INORGANIC CHEMISTRY COMMUNICATIONS	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=58195106300
3	Dr.A.Venkatesan	Two-Dimensional Layered Bismuthene/Antimonene Nanocomposite as a Potential Electrode Material for the Fabrication of High-Energy Density Hybrid Supercapacitors	ENERGY & FUELS	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57359869400
4	Dr.A.Venkatesan	Third Order Nonlinear Optical Properties of Bis (Creatininium 2,4-Dichlorobenzoate) Monohydrate Organic New Single Crystal	JOURNAL OF MOLECULAR STRUCTURE	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57359869400
5	Dr.S. Sakthivel	Molecular structure, electronic properties, ESP map (polar aprotic and polar protic solvents) and topology investigation on 1-(tert-Butoxycarbonyl)-3-piperidinecarboxylic acid-Anticancer therapeutic agent	JOURNAL OF MOLECULAR STRUCTURE	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57218539046

6	Dr.S. Sakthivel	The chemical reactivity and antimalarial investigation of crystal structure (2E)-3-(biphenyl-4-yl)-1-(4-chlorophenyl)prop-2-en-1-one and hydroxyphenyl, nitrophenyl substituted chalcone derivative molecules	JOURNAL OF MOLECULAR STRUCTURE	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57218539046
7	Dr.S. Sakthivel	Non-covalent interaction, adsorption characteristics and solvent effect of procainamide anti-arrhythmias drug on silver and gold loaded silica surfaces: SERS spectroscopy, density functional theory and molecular docking investigations	RSC ADVANCES	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57218539046
8	Dr.S. Sakthivel	Comparison of experimental and theoretical spectral groups, electronic properties, topological, and molecular docking investigations of 1-N-Cbz-piperidine-4-carboxylic acid- Potential Cancer drug	JOURNAL OF MOLECULAR STRUCTURE	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57218539046
9	Dr. C. Esther Jeyanthi	Impact of cobalt doping on magnetic and structural properties in Ce _{1-x} Co _x O ₂ (x = 0.1, 0.2 and 0.3) ceramics synthesized by combustion method	INORGANIC CHEMISTRY COMMUNICATIONS	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57218711789
10	Dr. C. Esther Jeyanthi	Fabrication, structural, thermo-mechanical and opto-electrical behavior of anthranilamide compound	Materials Today Communications / ISSN 2352-4928	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57218711789
11	Dr. S.Selvakumari	Vibrational spectroscopic, electronic influences, reactivity analysis and molecular docking studies of 2-Fluoro-4-iodo-5-methylpyridine	SPECTROSCOPY LETTERS	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079392
12	Dr. S.Selvakumari	Solvent - solute interactions, electronic properties, topological and biological explorations of 6-Bromo-7-methylimidazo[1,2-a]pyridine	JOURNAL OF MOLECULAR LIQUIDS	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079392

13	Dr. S.Selvakumari	Solvent effect on molecular, electronic parameters, topological analysis and Fukui function evaluation with biological studies of imidazo [1, 2-a]pyridine-8-carboxylic acid	JOURNAL OF MOLECULAR LIQUIDS	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079392
14	Dr. M. Vimala	Solvent role in molecular structure, thermodynamic quantities, reactions and electronic transitions (TDDFT) on 2-[piperidin-1-yl] phenol	JOURNAL OF MOLECULAR LIQUIDS	SCI/SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57223123757
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20	Dr.S.Bharanidharan	Synthesis, spectral characterisations of 3t- pentyl-2r,6c-diarylpiperidin-4-one oximepicrates:DFT studies and potent anti-microbial agents	MOLECULAR PHYSICS	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=56401203600
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22	Dr.S.Bharanidharan	Synthesis, Spectroscopic, Computational, Biological and Molecular docking studies on 3-allyl 2,6-diaryl piperidin-4-ones	CHEMISTRY SELECT	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=56401203600
23	Dr.S.Bharanidharan	Synthesis, spectroscopic profiling, biological evaluation, DFT, molecular docking and mathematical studies of 3,5-diethyl-2r,6c-diphenylpiperidin-4-one picrate	MOLECULAR PHYSICS	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=56401203600
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30	Dr. B. Anna Benedict	Ellagic Acid as a Potential Inhibitor against the Nonstructural Protein NS3 Helicase of Zika Virus: A Molecular Modelling Study	Biomed Research International	SCOPUS	https://doi.org/10.1155/2022/2044577
31	Dr. B. Anna Benedict	Design of novel pyrimidine based remdesivir analogues with dual target specificity for SARS CoV-2: A computational approach	International Journal of Biological Macrocycles	SCOPUS	https://doi.org/10.1016/j.ijbiomac.2023.124443
32	Dr A. Kistan	Experimental Investigations on the Mechanical Characteristics of Natural Fiber Particle-Reinforced Polymer Composites under Cryogenic Environment	Journal of Nanomaterials	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=56771385900&origin=recordpage
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35	Dr A. Kistan	Study on flexural behavior of polypropylene fiber reinforced fly ash concrete beam	Materials Today: Proceedings	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=56771385900&origin=recordpage

36	Dr. A. Kistan	Impact of cobalt doping on magnetic and structural properties in $\text{Ce}_{1-x}\text{Co}_x\text{O}_2$ ($x = 0.1, 0.2$ and 0.3) ceramics synthesized by Combustion method	Inorganic Chem. Communications	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=56771385900&origin=recordpage
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38	Dr. A. Saral	Experimental spectral Investigations for Structural, Electronic, Topological Properties and Molecular Docking studies of 2-Cyclohexylidene hydrazine carboxamide	Journal of the Indian Chemical Society	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079850
39	Dr. A. Saral	Solvent polarity, structural and electronic properties with different solvents and biological studies of 3,3,5-triphenylfuran-2(3H)-one- cancers of the blood cells	Journal of Molecular liquids	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079850
40	Dr. A. Saral	Synthesis, structural and theoretical investigations on 3-diethyl 2-({4-[3-ethoxy-2-(ethoxycarbonyl)-3-oxo-2-phenylpropyl]-2,5-dimethylphenyl}methyl)-2-phenylpropanedioate	Journal of the Indian Chemical Society	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079850
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42	Dr. A. Saral	Molecular level solvent interaction (microscopic), electronic, covalent assembly (RDG, AIM & ELF), ADMET prediction and anti-cancer activity of 1-(4-Fluorophenyl)-1-propanone): Cytotoxic agent	Journal of Molecular Liquids	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079850

43	Dr. A. Saral	Electronic, intermolecular, quantum computational investigations, molecular docking and simulation studies of the potent antiviral drug EIDD-2801	Journal of the Indian Chemical Society	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57226079850
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50	Mrs. J. Sumathi	Efficient Fluoride Removal from Aqueous Solution Using Natural Adsorbent Such as Eugenia Jambolana: Equilibrium Isotherm Analysis and Influence of Anions	Main Group Chemistry	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57202133816
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57	Dr. M. Sundar Raj	Unstable stream past an Improved monotonic infinite inclined plate with inconsistent Temperature and constant mass diffusion	Neuroquantology	SCOPUS	https://www.scopus.com/authid/detail.uri?authorId=57237620600
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