

Name of the faculty : Prof. Dr. T.B. Pawar
Designation : Professor
Department : Chemistry
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Details of Research Publications

Sr. No.	Title of the paper	Name of Journal	Year of publication	ISSN number	DOI/Online link
1.	Exploration of photocatalytic performance of TiO ₂ , Ni-doped TiO ₂ , and Fe-doped TiO ₂ for degradation of eosine blue dye: comparative study	Results in Chemistry	2022	2211-7156	https://www.scopus.com/sourceid/21101024415
2.	Synthesis, molecular structure, electronic, spectroscopic, NLO and antimicrobial study of N-benzyl-2-(5-aryl-1, 3, 4-oxadiazol-2-yl) aniline derivatives	Journal of Molecular Structure	2022	0022-2860	https://www.scopus.com/sourceid/24642
3.	Synthesis and characterization of ZnO/CuO nanocomposites as an effective photocatalyst and gas sensor for environmental remediation	Journal of Inorganic and Organometallic Polymers and Materials	2022	1574-1443	https://www.scopus.com/sourceid/4700152855
4.	Photocatalytic Applications of Doped Fe ₃ O ₄ Nanoparticles for Degradation of Methyl Orange and Methylene Blue Dyes: A Review	Asian Journal of Organic & Medicinal Chemistry	2022	2456-8937	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList
5.	Synthesis, Molecular Structure, HOMO-LUMO, Spectroscopic (UV-Vis and IR), Thermochemical Study of 5-Acetyl-4-(4-chlorophenyl)-6-methyl- 3,4-dihydropyrimidin-2(1H)-one: A DFT Study	Asian Journal of Organic & Medicinal Chemistry	2022	2456-8937	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList

6.	Spectroscopic (FTIR and UV), quantum Chemical, antifungal and antioxidant investigations of (E)-7-(4-(trifluoromethyl)benzylidene)-1, 2, 6, 7-tetrahydro-8H-indeno [5, 4-b] furan-8-one: A combined experimental and theoretical study	Vietnam Journal of Chemistry	2021	2572-8288	https://www.scopus.com/sourceid/21101043786
7.	Transition metals Fe ³⁺ , Ni ²⁺ modified titanium dioxide (TiO ₂) film sensors fabricated by CPT method to sense some toxic environmental pollutant gases	Journal of the Indian Chemical Society	2021	0019-4522	https://www.scopus.com/sourceid/24097
8.	Microwave prompted solvent-free synthesis of new series of heterocyclic tagged 7- arylidene indanone hybrids and their computational, antifungal, antioxidant, and cytotoxicity study	Bioorganic Chemistry	2021	0045-2068	https://www.scopus.com/sourceid/25789
9.	Superfast synthesis, antibacterial and antifungal studies of halo-aryl and heterocyclic tagged 2, 3-dihydro-1H-inden-1-one candidates	Monatshefte für Chemie-Chemical Monthly	2021	0026-9247	https://www.scopus.com/sourceid/24803
10.	DFT computational insights into structural, electronic and spectroscopic parameters of 2-(2-Hydrazineyl) thiazole derivatives: a concise theoretical and experimental approach	Journal of Sulfur Chemistry	2021	1741-5993	https://www.scopus.com/sourceid/24655
11.	Design, fabrication, antitubercular, antibacterial, antifungal and antioxidant study of silver doped ZnO and CuO nano candidates: A comparative pharmacological study	Current Research in Green and Sustainable Chemistry	2021	2666-0865	https://www.scopus.com/sourceid/21101043776
12.	Experimental and theoretical exploration on single crystal, structural, and quantum chemical parameters of (E)-7-(arylidene)-1, 2, 6, 7-tetrahydro-8 H-indeno [5, 4-b] furan-8-one derivatives: A comparative study	Journal of the Chinese Chemical Society	2021	0009-4536	https://www.scopus.com/sourceid/23449
13.	Density and Viscosity of LiCl, LiBr, LiI and KCl in Aqueous Methanol at 313.15 K	ORIENTAL JOURNAL OF CHEMISTRY	2021	0970-020X	https://mjl.clarivate.com:/search-results?issn=0970-020X&hide_exact_match.fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-

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14.	Solvent-free grindstone synthesis of four new (E)-7-(arylidene)-indanones and their structural, spectroscopic and quantum chemical study: a comprehensive theoretical and experimental exploration	Molecular Simulation	2020	0892-7022	https://www.scopus.com/sourceid/24801
15.	Molecular structure, frontier molecular orbital and spectroscopic examination on dihydropyrimidinones: a comparative computational approach	Journal of Advanced Scientific Research	2020	0976-9595	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList
16.	Efficient synthesis, antibacterial, antifungal, antioxidant and cytotoxicity study of 2-(2-hydrazineyl) thiazole derivatives	ChemistrySelect	2020	2365-6549	https://www.scopus.com/sourceid/21100850505
17.	Aqua-mediated rapid and benign synthesis of 1, 2, 6, 7-tetrahydro-8H-indeno [5, 4-b] furan-8-one-appended novel 2-arylidene indanones of pharmacological interest at ambient temperature	Journal of the Chinese Chemical Society	2020	0009-4536	https://www.scopus.com/sourceid/23449
18.	Transition metals Ni ²⁺ , Fe ³⁺ incorporated modified ZnO thick film sensors to monitor the environmental and industrial pollutant gases	ORIENTAL JOURNAL OF CHEMISTRY	2020	0970-020X	https://mjl.clarivate.com/search-results?issn=0970-020X&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal
19.	Molecular structure, electronic, chemical and spectroscopic (UV-visible and IR) studies of 5-(4-chlorophenyl)-3-(3, 4-dimethoxyphenyl)-1-phenyl-4, 5-dihydro-1H-pyrazole: combined DFT and experimental exploration	Material Science Research India	2020	0973-3469	Only peer reviewed journal

20.	Molecular structure, frontier molecular orbitals, MESP and UV-visible spectroscopy studies of Ethyl 4-(3, 4-dimethoxyphenyl)-6-methyl-2-oxo-1, 2, 3, 4-tetrahydropyrimidine-5-carboxylate: A theoretical and experimental appraisal	Material Science Research India	2020	0973-3469	Only peer reviewed journal
21.	Efficient synthesis, spectroscopic and quantum chemical study of 2, 3-dihydrobenzofuran labelled two novel arylidene indanones: A comparative theoretical exploration	Material Science Research India	2020	0973-3469	Only peer reviewed journal
22.	Experimental and Theoretical Studies on the Molecular Structure, FT-IR, NMR, HOMO, LUMO, MESP, and Reactivity Descriptors of (E)-1-(2, 3-Dihydrobenzo [b][1, 4] dioxin-6-yl)-3-(3, 4, 5-trimethoxyphenyl) prop-2-en-1-one	Material Science Research India	2020	0973-3469	Only peer reviewed journal
23.	Computational insights on molecular structure, electronic properties, and chemical reactivity of (E)-3-(4-chlorophenyl)-1-(2-hydroxyphenyl) prop-2-en-1-one	Material Science Research India	2020	0973-3469	Only peer reviewed journal
24.	Investigation of Structural and Spectroscopic Parameters of Ethyl 4-(4-isopropylphenyl)-6-methyl-2-oxo-1, 2, 3, 4-tetrahydropyrimidine-5-carboxylate: a DFT Study	Chemistry & Biology Interface	2020	2249-4820	https://ugccare.unipune.ac.in/Apps1/User/WebA/AlphabetwiseList?alphabet=C
25.	Synthesis, Molecular Structure, HOMOLUMO and Spectroscopic Investigation of (E)-1-(2,4-Dichloro-5-fluorophenyl)-3-(2,6-dichlorophenyl)prop-2-en-1-one: A DFT Based Computational Exploration	Asian Journal of Organic & Medicinal Chemistry	2020	2456-8937	https://ugccare.unipune.ac.in/Apps1/User/WebA/SearchList
26.	Ultrasound promoted stereoselective synthesis of 2, 3-dihydrobenzofuran appended chalcones at ambient temperature	South African Journal of Chemistry	2020	0379-4350	https://www.scopus.com/sourceid/21544
27.	Exploration of catalytic performance of nano-La2O3 as an efficient catalyst for dihydropyrimidinone/thione synthesis and gas sensing	Journal of Nanostructure in Chemistry	2019	2008-9244	https://mjl.clarivate.com/search-results?issn=2008-9244&hide_exact_match_fl=true&utm_source=mjl&utm_medium=share-by-link&utm_campaign=search-results-share-this-journal

28.	DFT Studies of 2-[(2-substitutedphenyl) carbamoyl] benzoic acids	Journal of Chemical, Biological and Physical Sciences	2017	2249-1929	UGC Approved List
29.	Poly (ethylene glycol)(PEG-400): A green approach towards synthesis of novel pyrazolo [3, 4-d] pyrimidin-6-amines derivatives and their antimicrobial screening	Archives of Applied Science Research	2014	0975-508X	UGC Approved List