

Asli Esme

List of Publications by Year in descending order

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papers

347
citations

933447

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839539

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23
docs citations

23
times ranked

338
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical and vibrational studies of 4,5-diphenyl-2-oxazole propionic acid (oxaprozin). <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 75, 1370-1376.	3.9	66
2	The vibrational studies and theoretical investigation of structure, electronic and non-linear optical properties of Sudan III [1-{[4-(phenylazo) phenyl]azo}-2-naphthalenol]. <i>Journal of Molecular Structure</i> , 2013, 1048, 185-195.	3.6	51
3	Spectroscopic (FT-IR, FT-Raman, UV-Vis) analysis, conformational, HOMO-LUMO, NBO and NLO calculations on monomeric and dimeric structures of 4-pyridazinecarboxylic acid by HF and DFT methods. <i>Journal of Molecular Structure</i> , 2017, 1147, 322-334.	3.6	50
4	Molecular structures, spectroscopic (FT-IR, NMR, UV) studies, NBO analysis and NLO properties for tautomeric forms of 1,3-dimethyl-5-(phenylazo)-6-aminouracil by density functional method. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 443-455.	3.9	46
5	Theoretical study on the relationship between the molecular structure and corrosion inhibition efficiency of long alkyl side chain acetamide and isoxazolidine derivatives. <i>Protection of Metals and Physical Chemistry of Surfaces</i> , 2012, 48, 710-721.	1.1	17
6	Conformational, spectroscopic (FT-IR, FT-Raman, and UV-Vis), and molecular docking studies of N-(2-hydroxyethyl) succinimide. <i>Journal of Molecular Structure</i> , 2019, 1195, 451-461.	3.6	17
7	Chemical reactivities and molecular docking studies of parthenolide with the main protease of HEP-G2 and SARS-CoV-2. <i>Journal of Molecular Structure</i> , 2021, 1243, 130705.	3.6	17
8	Mpro-SARS-CoV-2 Inhibitors and Various Chemical Reactivity of 1-Bromo- and 1-Chloro-4-vinylbenzene in [3 + 2] Cycloaddition Reactions. <i>Organics</i> , 2021, 2, 1-16.	1.3	16
9	Theoretical Studies of Molecular Structures, Infrared Spectra, NBO and NLO Properties of Some Novel 5-aryloxy-6-hydroxy-4-phenyl-3-cyano-2-pyridone Dyes. <i>Acta Physica Polonica A</i> , 2016, 130, 1273-1287.	0.5	15
10	Theoretical and spectroscopic studies of a tricyclic antidepressant, imipramine hydrochloride. <i>Journal of Molecular Structure</i> , 2018, 1161, 169-184.	3.6	12
11	Divulging the various chemical reactivity of trifluoromethyl-4-vinyl-benzene as well as methyl-4-vinyl-benzene in [3+2] cycloaddition reactions. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 102, 107760.	2.4	10
12	Divulging the regioselectivity of epoxides in the ring-opening reaction, and potential himachalene derivatives predicted to target the antibacterial activities and SARS-CoV-2 spike protein with docking study. <i>Journal of Molecular Structure</i> , 2021, 1244, 130864.	3.6	10
13	Experimental and theoretical studies on Sudan Red G [1-(2-methoxyphenylazo)-2-naphthol] and its Cu(II) coordination compound. <i>Journal of Molecular Structure</i> , 2014, 1075, 264-278.	3.6	9
14	Spectroscopic calculations, Hirshfeld surface analysis, and molecular docking studies of anticancer 6-(4-Aminophenyl)-4-(4-methoxyphenyl)-2-methoxynicotinonitrile. <i>Spectroscopy Letters</i> , 2021, 54, 51-64.	1.0	3
15	Synthesis of 4-(4-ethyl-phenyl)-3-(4-methyl-phenyl)-1,2,4-oxadiazol-5(4H)-one and 4-(4-ethyl-phenyl)-3-(4-methyl-phenyl)-1,2,4-oxadiazole-5(4H)-thione and solvent effects on their infrared spectra in organic solvents. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 251, 119424.	3.9	3
16	Theoretical Investigation on the Molecular Structure, Electronic, Spectroscopic Studies and Nonlinear Optical Properties of 5-bromo-1-(2-cyano-pyridin-4-yl)-1H-indazole-3-carboxylic acid diethylamide: a DFT and TD-DFT Study. <i>Acta Physica Polonica A</i> , 2019, 136, 378-394.	0.5	2
17	Quantum chemical calculations, Hirshfeld surface analysis, and molecular docking studies of antibacterial (E)-N-((1H-Indol-3-yl)methylene)-4-bromobenzohydrazide. <i>Spectroscopy Letters</i> , 2019, 52, 398-412.	1.0	1
18	The Crystal Structure, Spectral, and Density Functional Theory Studies of [3-(3-Bromophenyl)-cis-4,5-Dihydroisoxazole-4,5-Diyl]bis(Methylene)Diacetate. <i>Journal of Applied Spectroscopy</i> , 2021, 88, 633.	0.7	1

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19	Structural, spectral characterization, and topological study of (E)-5-(diethylamino)-2-((3,5-dinitrophenylimino)methyl)phenol. Structural Chemistry, 2023, 34, 455-466.	2.0	1
20	Quantum Chemical Calculations of the Spectroscopic Properties and Nonlinear Optical Activity of 2,6-Dibromo-3-Chloro-4-Fluoroaniline. Journal of Applied Spectroscopy, 2018, 84, 1098-1107.	0.7	0
21	Spectroscopic, Hirshfeld Surface Analysis, and Molecular Docking Studies on Potent Anti-inflammatory and Analgesic Activity Methyl 3-((pyridin-2-ylcarbonyl)amino)Benzoate. ChemistrySelect, 2020, 5, 3144-3158.	1.5	0
22	EXPERIMENTAL AND THEORETICAL STUDY OF THE SUBSTITUENT TYPE AND POSITION EFFECTS ON 3-(SUBSTITUTED-PHENYL)-CIS-(4,5-DIHYDROISOXAZOLE- 4,5-DIYL)BIS(METHYLENE)DIACETATE DERIVATIVES. Journal of Structural Chemistry, 2021, 62, 865-875.	1.0	0
23	Molecular Docking, Topological Analysis and Vibrational Studies on N-(2-Bromoethyl) Succinimide: Antidepressant Agent. Letters in Organic Chemistry, 2021, 18, 797-811.	0.5	0