Stevan ArmakoviÄ

List of Publications by Year
in descending order

134 papers	3,330 citations	109321 35 h-index	233421 45 g-index
140 all docs	140 docs citations	140 times ranked	1855 citing authors

#	Article	IF	Citations
1	Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study. Arabian Journal of Chemistry, 2020, 13, 632-648.	4.9	97
2	Influence of electron acceptors on the kinetics of metoprolol photocatalytic degradation in TiO₂ suspension. A combined experimental and theoretical study. RSC Advances, 2015, 5, 54589-54604.	3.6	95
3	Synthesis and spectroscopic study of three new oxadiazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential. Journal of Molecular Structure, 2018, 1173, 469-480.	3.6	83
4	Computational evaluation of the reactivity and pharmaceutical potential of an organic amine: A DFT, molecular dynamics simulations and molecular docking approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 222, 117188.	3.9	80
5	Synthesis, spectroscopic characterization, reactive properties by DFT calculations, molecular dynamics simulations and biological evaluation of Schiff bases tethered 1,2,4-triazole and pyrazole rings. Journal of Molecular Structure, 2019, 1177, 47-54.	3.6	71
6	Exploring the detailed spectroscopic characteristics, chemical and biological activity of two cyanopyrazine-2-carboxamide derivatives using experimental and theoretical tools. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 224, 117414.	3.9	69
7	Active components of frequently used Î²-blockers from the aspect of computational study. Journal of Molecular Modeling, 2012, 18, 4491-4501.	1.8	61
8	Synthesis and spectroscopic study of two new pyrazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential. Journal of Molecular Structure, 2019, 1181, 599-612.	3.6	59
9	Hydrogen storage properties of sumanene. International Journal of Hydrogen Energy, 2013, 38, 12190-12198.	7.1	57
10	Understanding reactivity of two newly synthetized imidazole derivatives by spectroscopic characterization and computational study. Journal of Molecular Structure, 2018, 1158, 176-196.	3.6	56
11	Aromaticity, response, and nonlinear optical properties of sumanene modified with boron and nitrogen atoms. Journal of Molecular Modeling, 2014, 20, 2538.	1.8	55
12	Efficiency of La-doped TiO2 calcined at different temperatures in photocatalytic degradation of Î²-blockers. Arabian Journal of Chemistry, 2019, 12, 5355-5369.	4.9	54
13	Optoelectronic properties of curved carbon systems. Carbon, 2017, 111, 371-379.	10.3	53
14	Synthesis, XRD crystal structure, spectroscopic characterization (FT-IR, 1H and 13C NMR), DFT studies, chemical reactivity and bond dissociation energy studies using molecular dynamics simulations and evaluation of antimicrobial and antioxidant activities of a novel chalcone derivative, (E)-1-(4-bromophenyl)-3-(4-iodophenyl)prop-2-en-1-one. Journal of Molecular Structure, 2017, 1128, 520-533.	3.6	53
15	Molecular dynamic simulations, ALIE surface, Fukui functions geometrical, molecular docking and vibrational spectra studies of tetra chloro p and m-xylene. Journal of Molecular Structure, 2018, 1171, 253-267.	3.6	53
16	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. Journal of Molecular Structure, 2020, 1205, 127587.	3.6	53
17	Stability and reactivity study of bio-molecules brucine and colchicine towards electrophile and nucleophile attacks: Insight from DFT and MD simulations. Journal of Molecular Liquids, 2021, 335, 116192.	4.9	53
18	A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene â€“ A frequently used benzene derivative. Journal of Molecular Structure, 2018, 1151, 245-255.	3.6	51

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19	Spectroscopic analysis and molecular docking of imidazole derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations. Journal of Molecular Structure, 2018, 1158, 156-175.	3.6	49
20	Investigation of spectroscopic, reactive, transport and docking properties of 1-(3,4-dichlorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea (ANF-6): Combined experimental and computational study. Journal of Molecular Structure, 2017, 1134, 668-680.	3.6	48
21	Synthesis, characterization and computational studies of semicarbazide derivative. Journal of Molecular Liquids, 2018, 272, 481-495.	4.9	48
22	Optical and bowl-to-bowl inversion properties of sumanene substituted on its benzylic positions; a DFT/TD-DFT study. Chemical Physics Letters, 2013, 578, 156-161.	2.6	47
23	Hybrid and bioactive cocrystals of pyrazinamide with hydroxybenzoic acids: Detailed study of structure, spectroscopic characteristics, other potential applications and noncovalent interactions using SAPT. Journal of Molecular Structure, 2020, 1202, 127316.	3.6	47
24	Sumanene and its adsorption properties towards CO, CO2 and NH3 molecules. Journal of Molecular Modeling, 2014, 20, 2170.	1.8	46
25	Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea. RSC Advances, 2016, 6, 111997-112015.	3.6	46
26	FT-IR, FT-Raman and NMR characterization of 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate and investigation of its reactive and optoelectronic properties by molecular dynamics simulations and DFT calculations. Journal of Molecular Structure, 2017, 1127, 124-137.	3.6	46
27	Synthesis, characterization and computational study of the newly synthetized sulfonamide molecule. Journal of Molecular Structure, 2018, 1153, 212-229.	3.6	46
28	Synthesis of 5-(5-methyl-benzofuran-3-ylmethyl)-3H- [1, 3, 4] oxadiazole-2-thione and investigation of its spectroscopic, reactivity, optoelectronic and drug likeness properties by combined computational and experimental approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 205, 95-110.	3.9	45
29	Theoretical Studies on the Structure and Various Physico-Chemical and Biological Properties of a Terphenyl Derivative with Immense Anti-Protozoan Activity. Polycyclic Aromatic Compounds, 2021, 41, 825-840.	2.6	44
30	Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures. Journal of Molecular Structure, 2017, 1141, 495-511.	3.6	43
31	Structural, spectroscopic characterization of 2-(5-methyl-1-benzofuran-3-yl) acetic acid in monomer, dimer and identification of specific reactive, drug likeness properties: Experimental and computational study. Journal of Molecular Structure, 2019, 1178, 1-17.	3.6	43
32	Influence of sumanene modifications with boron and nitrogen atoms to its hydrogen adsorption properties. Physical Chemistry Chemical Physics, 2016, 18, 2859-2870.	2.8	42
33	Structuring of water in the new generation ionic liquid â€“ Comparative experimental and theoretical study. Journal of Chemical Thermodynamics, 2016, 93, 164-171.	2.0	42
34	Spectroscopic, DFT, molecular dynamics and molecular docking study of 1-butyl-2-(4-hydroxyphenyl)-4,5-dimethyl-imidazole 3-oxide. Journal of Molecular Structure, 2017, 1134, 330-344.	3.6	42
35	Spectroscopic analysis of 8-hydroxyquinoline derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations. Journal of Molecular Structure, 2018, 1156, 336-347.	3.6	42
36	Concentration and solvent dependent SERS, DFT, MD simulations and molecular docking studies of a thioxothiazolidine derivative with antimicrobial properties. Journal of Molecular Liquids, 2021, 329, 115582.	4.9	40

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37	Theoretical investigation of loratadine reactivity in order to understand its degradation properties: DFT and MD study. Journal of Molecular Modeling, 2016, 22, 240.	1.8	39
38	Spectroscopic characterization of 1-[3-(1 H -imidazol-1-yl)propyl]-3-phenylthiourea and assessment of reactive and optoelectronic properties employing DFT calculations and molecular dynamics simulations. Journal of Molecular Structure, 2017, 1129, 72-85.	3.6	39
39	Vibrational spectroscopic analysis of cyanopyrazine-2-carboxamide derivatives and investigation of their reactive properties by DFT calculations and molecular dynamics simulations. Journal of Molecular Structure, 2017, 1131, 1-15.	3.6	35
40	Vibrational and electronic absorption spectroscopic profiling, natural hybrid orbital, charge transfer, electron localization function and molecular docking analysis on 3-amino-3-(2-nitrophenyl) propionic acid. Journal of Molecular Structure, 2018, 1171, 733-746.	3.6	32
41	Structure making properties of 1-(2-hydroxylethyl)-3-methylimidazolium chloride ionic liquid. Journal of Chemical Thermodynamics, 2016, 95, 174-179.	2.0	30
42	Spectroscopic profiling (FT-IR, FT-Raman, NMR and UV-Vis), autoxidation mechanism (H-BDE) and molecular docking investigation of 3-(4-chlorophenyl)-N,N-dimethyl-3-pyridin-2-ylpropan-1-amine by DFT/TD-DFT and molecular dynamics: A potential SSRI drug. Computational Biology and Chemistry, 2018, 77, 131-145.	2.3	29
43	An analysis of structural and spectroscopic signatures, the reactivity study of synthetized 4,6-dichloro-2-(methylsulfonyl)pyrimidine: A potential third-order nonlinear optical material. Journal of Molecular Structure, 2019, 1186, 263-275.	3.6	27
44	Spectroscopic characterization of 4-[2-(5-Ethylpyridin-2-yl)ethoxy]benzaldehyde oxime and investigation of its reactive properties by DFT calculations and molecular dynamics simulations. Journal of Molecular Structure, 2017, 1128, 245-256.	3.6	26
45	Molecular structure, optoelectronic properties, spectroscopic (FT-IR, FT-Raman and UVâ€“Vis), H-BDE, NBO and drug likeness investigations on 7, 8-benzocoumarin-4-acetic acid (7BAA). Journal of Molecular Structure, 2019, 1195, 815-826.	3.6	26
46	Fullerene C₂₄ as a potential carrier of ephedrine drug â€“ a computational study of interactions and influence of temperature. Physical Chemistry Chemical Physics, 2019, 21, 23329-23337.	2.8	26
47	Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuron. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117580.	3.9	26
48	Self-assembling, reactivity and molecular dynamics of fullerenol nanoparticles. Physical Chemistry Chemical Physics, 2017, 19, 135-144.	2.8	25
49	Photocatalytic degradation of 4-amino-6-chlorobenzene-1,3-disulfonamide stable hydrolysis product of hydrochlorothiazide: Detection of intermediates and their toxicity. Environmental Pollution, 2018, 233, 916-924.	7.5	23
50	Experimental and computational study of hydrolysis and photolysis of antibiotic ceftriaxone: Degradation kinetics, pathways, and toxicity. Science of the Total Environment, 2021, 768, 144991.	8.0	23
51	Determination of reactive properties of 1-butyl-3-methylimidazolium taurate ionic liquid employing DFT calculations. Journal of Molecular Liquids, 2016, 222, 796-803.	4.9	22
52	Spectroscopic analysis of 8-hydroxyquinoline-5-sulphonic acid and investigation of its reactive properties by DFT and molecular dynamics simulations. Journal of Molecular Structure, 2017, 1150, 540-552.	3.6	22
53	Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of Nâ€²-diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide. Journal of Molecular Structure, 2017, 1130, 208-222.	3.6	22
54	Interactions of Schiff base compounds and their coordination complexes with the drug cisplatin. New Journal of Chemistry, 2018, 42, 5834-5843.	2.8	22

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55	Spectroscopic characterization of hydroxyquinoline derivatives with bromine and iodine atoms and theoretical investigation by DFT calculations, MD simulations and molecular docking studies. Journal of Molecular Structure, 2018, 1167, 95-106.	3.6	22
56	Specificities of boron disubstituted sumanenes. Journal of Molecular Modeling, 2013, 19, 1153-1166.	1.8	21
57	Remarkable colorimetric sensing behavior of pyrazole-based chemosensor towards Cu(<scp>ii</scp>) ion detection: synthesis, characterization and theoretical investigations. RSC Advances, 2018, 8, 18023-18029.	3.6	21
58	Investigation of the reactivity properties of a thiourea derivative with anticancer activity by DFT and MD simulations. Journal of Molecular Modeling, 2021, 27, 217.	1.8	21
59	FT-IR and FT-Raman characterization and investigation of reactive properties of N-(3-iodo-4-methylphenyl)pyrazine-2-carboxamide by molecular dynamics simulations and DFT calculations. Journal of Molecular Structure, 2017, 1136, 14-24.	3.6	20
60	Synthesis, crystal structure analysis, spectral investigations, DFTÂcomputations and molecular dynamics and docking study of 4-benzyl-5-oxomorpholine-3-carbamide, a potential bioactive agent. Journal of Molecular Structure, 2017, 1134, 25-39.	3.6	20
61	Optoelectronic properties of the newly designed 1,3,5-triazine derivatives with isatin, chalcone and acridone moieties. Computational and Theoretical Chemistry, 2021, 1197, 113160.	2.5	20
62	Sumanene as a delivery system for 5-fluorouracil drug â€“ DFT, SAPT and MD study. Journal of Molecular Liquids, 2021, 342, 117526.	4.9	20
63	Synthesis, spectroscopic analyses (FT-IR and NMR), vibrational study, chemical reactivity and molecular docking study and anti-tubercular activity of condensed oxadiazole and pyrazine derivatives. Journal of Molecular Structure, 2018, 1156, 657-674.	3.6	19
64	Coordination compounds of a hydrazone derivative with Co(<scp>iii</scp>), Ni(<scp>ii</scp>), Cu(<scp>ii</scp>) and Zn(<scp>ii</scp>): synthesis, characterization, reactivity assessment and biological evaluation. New Journal of Chemistry, 2016, 40, 5885-5895.	2.8	18
65	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. Journal of Molecular Structure, 2017, 1135, 1-14.	3.6	18
66	Synthesis, XRD single crystal structure analysis, vibrational spectral analysis, molecular dynamics and molecular docking studies of 2-(3-methoxy-4-hydroxyphenyl) benzothiazole. Journal of Molecular Structure, 2017, 1148, 282-292.	3.6	18
67	Synthesis, spectroscopic analyses, chemical reactivity and molecular docking study and anti-tubercular activity of pyrazine and condensed oxadiazole derivatives. Journal of Molecular Structure, 2018, 1164, 459-469.	3.6	18
68	Structural, antioxidant, antiproliferative and inâ€'silico study of pyridine-based hydrazonylâ€'selenazoles and their sulphur isosteres. Journal of Molecular Structure, 2021, 1240, 130512.	3.6	18
69	Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative. Journal of Molecular Structure, 2019, 1176, 881-894.	3.6	17
70	DFT study of 1-butyl-3-methylimidazolium salicylate: a third-generation ionic liquid. Journal of Molecular Modeling, 2015, 21, 246.	1.8	16
71	Kosmotropism of newly synthesized 1-butyl-3-methylimidazolium taurate ionic liquid: Experimental and computational study. Journal of Chemical Thermodynamics, 2016, 94, 85-95.	2.0	16
72	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. Journal of Molecular Structure, 2018, 1155, 184-195.	3.6	16

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73	Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione. Journal of Molecular Structure, 2019, 1175, 269-279.	3.6	16
74	Reactivity properties and adsorption behavior of a triazole derivative â€“ DFT and MD simulation studies. Journal of Molecular Liquids, 2021, 341, 117439.	4.9	16
75	Investigation of boron modified graphene nanostructures; optoelectronic properties of graphene nanoparticles and transport properties of graphene nanosheets. Journal of Physics and Chemistry of Solids, 2016, 98, 156-166.	4.0	15
76	Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxymethyl benzimidazole. Journal of Molecular Structure, 2017, 1129, 86-97.	3.6	15
77	A DFT and MD study of reactive, H2 adsorption and optoelectronic properties of graphane nanoparticles â€“ An influence of boron doping. Materials Chemistry and Physics, 2020, 241, 122329.	4.0	15
78	Electronic structure of yttrium-doped zinc ferrite â€“ Insights from experiment and theory. Journal of Alloys and Compounds, 2020, 842, 155704.	5.5	15
79	Studies on the synthesis, spectroscopic analysis, molecular docking and DFT calculations on 1-hydroxy-2-(4-hydroxyphenyl)-4,5-dimethyl-imidazol 3-oxide. Journal of Molecular Structure, 2017, 1130, 644-658.	3.6	14
80	Reactive, spectroscopic and antimicrobial assessments of 5-[(4-methylphenyl) acetamido]-2-(4-tert-butylphenyl)benzoxazole: Combined experimental and computational study. Journal of Molecular Structure, 2017, 1128, 694-706.	3.6	14
81	Design, synthesis and computational analysis of novel acridine-(sulfadiazine/sulfathiazole) hybrids as antibacterial agents. Journal of Molecular Structure, 2019, 1186, 39-49.	3.6	14
82	Kinetics, mechanism and toxicity of intermediates of solar light induced photocatalytic degradation of pindolol: Experimental and computational modeling approach. Journal of Hazardous Materials, 2020, 393, 122490.	12.4	14
83	Biomass waste utilization for adsorbent preparation in CO2 capture and sustainable environment applications. Sustainable Energy Technologies and Assessments, 2021, 46, 101288.	2.7	14
84	Insight into the reactive properties of newly synthesized 1,2,4-triazole derivative by combined experimental (FT-IR and FR-Raman) and theoretical (DFT and MD) study. Journal of Molecular Structure, 2017, 1141, 542-550.	3.6	13
85	Optoelectronic and charge carrier hopping properties of ultra-thin boron nitride nanotubes. Superlattices and Microstructures, 2015, 79, 79-85.	3.1	12
86	Investigation of 1,2,3-trialkylimidazolium ionic liquids: experiment and density functional theory calculations. New Journal of Chemistry, 2017, 41, 650-660.	2.8	12
87	Uncommon structure making/breaking behaviour of cholinium taurate in water. Journal of Chemical Thermodynamics, 2017, 107, 58-64.	2.0	12
88	Pyridoxylidene aminoguanidine and its copper(II) complexes â€“ Syntheses, structure, and DFT calculations. Journal of Coordination Chemistry, 2017, 70, 2870-2887.	2.2	12
89	Adsorption properties of graphene towards the ephedrine â€“ A frequently used molecule in sport. Computational and Theoretical Chemistry, 2018, 1124, 39-50.	2.5	12
90	Understanding how yttrium doping influences the properties of nickel ferrite â€“ Combined experimental and computational study. Ceramics International, 2019, 45, 20290-20296.	4.8	12

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91	4-[(4-acetylphenyl)amino]-2-methylidene-4-oxobutanoic acid, a newly synthesized amide with hydrophilic and hydrophobic segments: Spectroscopic characterization and investigation of its reactive properties. Journal of the Serbian Chemical Society, 2018, 83, 1-18.	0.8	12
92	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. Journal of Molecular Structure, 2017, 1134, 814-827.	3.6	11
93	Synthesis, XRD crystal structure, spectroscopic characterization, local reactive properties using DFT and molecular dynamics simulations and molecular docking study of (E)-1-(4-bromophenyl)-3-(4-(trifluoromethoxy)phenyl)prop-2-en-1-one. Journal of Molecular Structure, 2017, 1137, 419-430.	3.6	11
94	Conformational, vibrational and DFT studies of a newly synthesized arylpiperazine-based drug and evaluation of its reactivity towards the human GABA receptor. Journal of Molecular Structure, 2017, 1147, 266-280.	3.6	11
95	Structural and spectroscopic characterization, reactivity study and charge transfer analysis of the newly synthetized 2-(6-hydroxy-1-benzofuran-3-yl) acetic acid. Journal of Molecular Structure, 2018, 1162, 81-95.	3.6	11
96	Spectroscopic characterization of 8-hydroxy-5-nitroquinoline and 5-chloro-8-hydroxy quinoline and investigation of its reactive properties by DFT calculations and molecular dynamics simulations. Journal of Molecular Structure, 2018, 1164, 525-538.	3.6	11
97	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. Journal of Molecular Structure, 2017, 1137, 589-605.	3.6	10
98	Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1H-benzoimidazole.3H2O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies. Journal of Molecular Structure, 2017, 1149, 602-612.	3.6	10
99	Two novel imidazole derivatives â€“ Combined experimental and computational study. Journal of Molecular Structure, 2018, 1173, 221-239.	3.6	10
100	Photophysical properties and theoretical investigations of newly synthesized pyrene-naphthalene based Schiff base ligand and its copper(II) complexes. Inorganica Chimica Acta, 2019, 486, 698-703.	2.4	10
101	Understanding reactivity of a triazole derivative and its interaction with graphene and doped/undoped-coroneneâ€"a DFT study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2316-2326.	3.5	10
102	Investigation of reactive properties of an antiviral azatricyclo derivativeâ€“KDFT, MD and docking simulations. Journal of Molecular Structure, 2021, 1230, 129937.	3.6	10
103	Investigation of reactive properties, adsorption on fullerene, DFT, molecular dynamics simulation of an anthracene derivative targeting dihydrofolate reductase and human dUTPase. Journal of Biomolecular Structure and Dynamics, 2021, , 1-10.	3.5	10
104	The role of environmental waters ionic composition and UVâ€“LED radiation on photodegradation, mineralization and toxicity of commonly used Î²-blockers. Journal of Molecular Structure, 2022, 1249, 131579.	3.6	10
105	Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial studies and molecular dynamics study of 5-[(4-nitrophenyl)acetamido]-2-(4-tert-butylphenyl)benzoxazole. Journal of Molecular Structure, 2017, 1133, 557-573.	3.6	9
106	Indole moiety induced biological potency in pseudo-peptides derived from 2-amino-2-(1H-indole-2-yl) based acetamides: Chemical synthesis, inÂvitro anticancer activity and theoretical studies. Journal of Molecular Structure, 2020, 1217, 128445.	3.6	9
107	Tumoricidal Potential of Novel Amino-1,10-phenanthroline Derived Imine Ligands: Chemical Preparation, Structure, and Biological Investigations. Molecules, 2020, 25, 2865.	3.8	9
108	Optoelectronic properties of higher acenes, their BN analogue and substituted derivatives. Materials Chemistry and Physics, 2016, 170, 210-217.	4.0	8

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109	Molecular conformational analysis, reactivity, vibrational spectral analysis and molecular dynamics and docking studies of 6-chloro-5-isopropylpyrimidine-2,4(1H,3H)-dione, a potential precursor to bioactive agent. Journal of Molecular Structure, 2017, 1127, 427-436.	3.6	8
110	Complexes of Zn(II) and Cd(II) with 2-acetylpyridine -aminoguanidine â€“ Syntheses, structures and DFT calculations. Inorganica Chimica Acta, 2018, 473, 160-168.	2.4	8
111	Crystal structure determination and computational studies of 1,4-dihydropyridine derivatives as selective T-type calcium channel blockers. Journal of Molecular Structure, 2021, 1230, 129898.	3.6	8
112	PbSe sensitized with iodine and oxygen: a combined computational and experimental study. Journal of Alloys and Compounds, 2021, , 163119.	5.5	8
113	Optical properties of layers of symmetric molecular nanofilms. Journal of Optics (India), 2015, 44, 1-6.	1.7	7
114	Theoretical investigation on the reactivity and photophysical properties of cobalt(II) and manganese(II) complexes constructed using Schiff base ligands based on ALIE and TDDFT calculations. Polyhedron, 2017, 129, 141-148.	2.2	7
115	Synthesis, theoretical studies and molecular docking of a novel chlorinated tetracyclic: (Z/E)-3-(1,8-dichloro-9,10-dihydro-9,10-ethanoanthracen-11-yl)acrylaldehyde. Journal of Molecular Structure, 2017, 1150, 358-365.	3.6	7
116	SURFACE LOCALIZATION OF ELECTRONS IN ULTRATHIN CRYSTALLINE STRUCTURES. Modern Physics Letters B, 2014, 28, 1450023.	1.9	6
117	Spectroscopic and reactive properties of a newly synthesized quinazoline derivative: Combined experimental, DFT, molecular dynamics and docking study. Journal of Molecular Structure, 2017, 1134, 863-881.	3.6	6
118	Synthesis, crystal structure, Hirshfeld surface analysis, spectroscopic characterization, reactivity study by DFT and MD approaches and molecular docking study of a novel chalcone derivative. Journal of Molecular Structure, 2017, 1135, 234-246.	3.6	6
119	Structural, biological and in-silico study of quinoline-based chalcogensemicarbazones. Journal of Molecular Structure, 2020, 1203, 127482.	3.6	6
120	Linking azoles to isoniazid via hydrazone bridge: Synthesis, crystal structure determination, antitubercular evaluation and computational studies. Journal of Molecular Liquids, 2022, 354, 118873.	4.9	6
121	Investigation of reactive and spectroscopic properties of oxobutanoic acid derivative: Combined spectroscopic, DFT, MD and docking study. Journal of Molecular Structure, 2017, 1148, 266-275.	3.6	4
122	A computational study of polydimethylsiloxane derivatives as a semi-permeable membrane for in-field identification of naphthenic acids in water using portable mass spectrometry. Journal of Molecular Liquids, 2022, 351, 118657.	4.9	4
123	Novel synthetic approach, spectroscopic characterization and theoretical studies on global and local reactive properties of a bibenzimidazolyl derivative. Journal of Molecular Structure, 2017, 1147, 121-128.	3.6	3
124	Unprecedented copper(ii) coordination induced nucleophilic cleavage of a quinoxaline heterocycle: structural and computational studies. CrystEngComm, 2021, 23, 5078-5086.	2.6	3
125	Comprehensive Study of the Chemistry behind the Stability of Carboxylic SWCNT Dispersions in the Development of a Transparent Electrode. Nanomaterials, 2022, 12, 1901.	4.1	3
126	Modeling of fundamental electronic circuits by the Euler method using the Python programming language. Physics Education, 2020, 55, 055016.	0.5	2

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127	Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. Symmetry, 2021, 13, 1619.	2.2	2
128	Removal of hydrochlorothiazide from drinking and environmental water: Hydrolysis, direct and indirect photolysis. Energy and Environment, 0, , 0958305X2210840.	4.6	2
129	Spectroscopic investigations, DFT calculations, molecular docking and MD simulations of 3-[(4-Carboxyphenyl) carbamoyl]-4-hydroxy-2-oxo-1, 2-dihydroxy quinoline-6-carboxylic acid. Journal of Molecular Structure, 2022, 1264, 133315.	3.6	2
130	Changes in optical characteristics of dielectric nanofilm structures in relation to bulk ones. , 2012, , .		0
131	Synthesis, crystal structure analysis, molecular docking studies and density functional theory predictions of the local reactive properties and degradation properties of a novel halochalcone. Journal of Molecular Structure, 2017, 1144, 246-253.	3.6	0
132	Potential of Sumanene Modified with Boron and Nitrogen Atoms for Adsorption of Carbon Dioxide: DFT and SAPT Study. Proceedings (mdpi), 2019, 15, 28.	0.2	0
133	Particularities in physical characteristics of molecular crystalline nanofilms. Zbornik Matice Srpske Za Prirodne Nauke, 2010, , 115-125.	0.1	0
134	Structural and computational study of quinoline-based chalcogensemicarbazones. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e566-e566.	0.1	0