

# Stevan ArmakoviÄ

## List of Publications by Year in descending order

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134  
papers

3,330  
citations

109311

35  
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233409

45  
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140  
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140  
docs citations

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times ranked

1855  
citing authors

#	ARTICLE	IF	CITATIONS
1	Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study. <i>Arabian Journal of Chemistry</i> , 2020, 13, 632-648.	4.9	97
2	Influence of electron acceptors on the kinetics of metoprolol photocatalytic degradation in TiO <sub>2</sub> suspension. A combined experimental and theoretical study. <i>RSC Advances</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117414.	3.9	69
7	Active components of frequently used $\beta$ -blockers from the aspect of computational study. <i>Journal of Molecular Modeling</i> , 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. <i>Journal of Molecular Structure</i> , 2019, 1181, 599-612.	3.6	59
9	Hydrogen storage properties of sumanene. <i>International Journal of Hydrogen Energy</i> , 2013, 38, 12190-12198.	7.1	57
10	Understanding reactivity of two newly synthesized imidazole derivatives by spectroscopic characterization and computational study. <i>Journal of Molecular Structure</i> , 2018, 1158, 176-196.	3.6	56
11	Aromaticity, response, and nonlinear optical properties of sumanene modified with boron and nitrogen atoms. <i>Journal of Molecular Modeling</i> , 2014, 20, 2538.	1.8	55
12	Efficiency of La-doped TiO <sub>2</sub> calcined at different temperatures in photocatalytic degradation of $\beta$ -blockers. <i>Arabian Journal of Chemistry</i> , 2019, 12, 5355-5369.	4.9	54
13	Optoelectronic properties of curved carbon systems. <i>Carbon</i> , 2017, 111, 371-379.	10.3	53
14	Synthesis, XRD crystal structure, spectroscopic characterization (FT-IR, <sup>1</sup> H and <sup>13</sup> C 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2018, 1171, 253-267.	3.6	53
16	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Liquids</i> , 2021, 335, 116192.	4.9	53
18	A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene "A frequently used benzene derivative. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1134, 668-680.	3.6	48
21	Synthesis, characterization and computational studies of semicarbazide derivative. <i>Journal of Molecular Liquids</i> , 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. <i>Chemical Physics Letters</i> , 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. <i>Journal of Molecular Structure</i> , 2020, 1202, 127316.	3.6	47
24	Sumanene and its adsorption properties towards CO, CO <sub>2</sub> and NH <sub>3</sub> molecules. <i>Journal of Molecular Modeling</i> , 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. <i>RSC Advances</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1127, 124-137.	3.6	46
27	Synthesis, characterization and computational study of the newly synthesized sulfonamide molecule. <i>Journal of Molecular Structure</i> , 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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 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. <i>Polycyclic Aromatic Compounds</i> , 2021, 41, 825-840.	2.6	44
30	Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2019, 1178, 1-17.	3.6	43
32	Influence of sumanene modifications with boron and nitrogen atoms to its hydrogen adsorption properties. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 2859-2870.	2.8	42
33	Structuring of water in the new generation ionic liquid "Comparative experimental and theoretical study. <i>Journal of Chemical Thermodynamics</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Modeling</i> , 2016, 22, 240.	1.8	39
38	Spectroscopic characterization of 1-[3-(1H-imidazol-1-yl)propyl]-3-phenylthiourea and assessment of reactive and optoelectronic properties employing DFT calculations and molecular dynamics simulations. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2018, 1171, 733-746.	3.6	32
41	Structure making properties of 1-(2-hydroxyethyl)-3-methylimidazolium chloride ionic liquid. <i>Journal of Chemical Thermodynamics</i> , 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. <i>Computational Biology and Chemistry</i> , 2018, 77, 131-145.	2.3	29
43	An analysis of structural and spectroscopic signatures, the reactivity study of synthesized 4,6-dichloro-2-(methylsulfonyl)pyrimidine: A potential third-order nonlinear optical material. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1128, 245-256.	3.6	26
45	Molecular structure, optoelectronic properties, spectroscopic (FT-IR, FT-Raman and UV-Vis), H-BDE, NBO and drug likeness investigations on 7, 8-benzocoumarin-4-acetic acid (7BAA). <i>Journal of Molecular Structure</i> , 2019, 1195, 815-826.	3.6	26
46	Fullerene C <sub>24</sub> as a potential carrier of ephedrine drug – a computational study of interactions and influence of temperature. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 228, 117580.	3.9	26
48	Self-assembling, reactivity and molecular dynamics of fullerene nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 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. <i>Environmental Pollution</i> , 2018, 233, 916-924.	7.5	23
50	Experimental and computational study of hydrolysis and photolysis of antibiotic ceftriaxone: Degradation kinetics, pathways, and toxicity. <i>Science of the Total Environment</i> , 2021, 768, 144991.	8.0	23
51	Determination of reactive properties of 1-butyl-3-methylimidazolium taurate ionic liquid employing DFT calculations. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1150, 540-552.	3.6	22
53	Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of N <sup>2</sup> -diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide. <i>Journal of Molecular Structure</i> , 2017, 1130, 208-222.	3.6	22
54	Interactions of Schiff base compounds and their coordination complexes with the drug cisplatin. <i>New Journal of Chemistry</i> , 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. <i>Journal of Molecular Structure</i> , 2018, 1167, 95-106.	3.6	22
56	Specificities of boron disubstituted sumanenes. <i>Journal of Molecular Modeling</i> , 2013, 19, 1153-1166.	1.8	21
57	Remarkable colorimetric sensing behavior of pyrazole-based chemosensor towards Cu(II) ion detection: synthesis, characterization and theoretical investigations. <i>RSC Advances</i> , 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. <i>Journal of Molecular Modeling</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1136, 14-24.	3.6	20
60	Synthesis, crystal structure analysis, spectral investigations, DFT computations and molecular dynamics and docking study of 4-benzyl-5-oxomorpholine-3-carbamide, a potential bioactive agent. <i>Journal of Molecular Structure</i> , 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. <i>Computational and Theoretical Chemistry</i> , 2021, 1197, 113160.	2.5	20
62	Sumanene as a delivery system for 5-fluorouracil drug – DFT, SAPT and MD study. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Structure</i> , 2018, 1156, 657-674.	3.6	19
64	Coordination compounds of a hydrazone derivative with Co(III), Ni(II), Cu(II) and Zn(II): synthesis, characterization, reactivity assessment and biological evaluation. <i>New Journal of Chemistry</i> , 2016, 40, 5885-5895.	2.8	18
65	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2018, 1164, 459-469.	3.6	18
68	Structural, antioxidant, antiproliferative and in silico study of pyridine-based hydrazone-selenazoles and their sulphur isosteres. <i>Journal of Molecular Structure</i> , 2021, 1240, 130512.	3.6	18
69	Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative. <i>Journal of Molecular Structure</i> , 2019, 1176, 881-894.	3.6	17
70	DFT study of 1-butyl-3-methylimidazolium salicylate: a third-generation ionic liquid. <i>Journal of Molecular Modeling</i> , 2015, 21, 246.	1.8	16
71	Kosmotropism of newly synthesized 1-butyl-3-methylimidazolium taurate ionic liquid: Experimental and computational study. <i>Journal of Chemical Thermodynamics</i> , 2016, 94, 85-95.	2.0	16
72	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2019, 1175, 269-279.	3.6	16
74	Reactivity properties and adsorption behavior of a triazole derivative – DFT and MD simulation studies. <i>Journal of Molecular Liquids</i> , 2021, 341, 117439.	4.9	16
75	Investigation of boron modified graphene nanostructures; optoelectronic properties of graphene nanoparticles and transport properties of graphene nanosheets. <i>Journal of Physics and Chemistry of Solids</i> , 2016, 98, 156-166.	4.0	15
76	Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxyethyl benzimidazole. <i>Journal of Molecular Structure</i> , 2017, 1129, 86-97.	3.6	15
77	A DFT and MD study of reactive, H <sub>2</sub> adsorption and optoelectronic properties of graphene nanoparticles – An influence of boron doping. <i>Materials Chemistry and Physics</i> , 2020, 241, 122329.	4.0	15
78	Electronic structure of yttrium-doped zinc ferrite – Insights from experiment and theory. <i>Journal of Alloys and Compounds</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1128, 694-706.	3.6	14
81	Design, synthesis and computational analysis of novel acridine-(sulfadiazine/sulfathiazole) hybrids as antibacterial agents. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Hazardous Materials</i> , 2020, 393, 122490.	12.4	14
83	Biomass waste utilization for adsorbent preparation in CO <sub>2</sub> capture and sustainable environment applications. <i>Sustainable Energy Technologies and Assessments</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1141, 542-550.	3.6	13
85	Optoelectronic and charge carrier hopping properties of ultra-thin boron nitride nanotubes. <i>Superlattices and Microstructures</i> , 2015, 79, 79-85.	3.1	12
86	Investigation of 1,2,3-trialkylimidazolium ionic liquids: experiment and density functional theory calculations. <i>New Journal of Chemistry</i> , 2017, 41, 650-660.	2.8	12
87	Uncommon structure making/breaking behaviour of cholinium taurate in water. <i>Journal of Chemical Thermodynamics</i> , 2017, 107, 58-64.	2.0	12
88	Pyridoxylidene aminoguanidine and its copper(II) complexes – Syntheses, structure, and DFT calculations. <i>Journal of Coordination Chemistry</i> , 2017, 70, 2870-2887.	2.2	12
89	Adsorption properties of graphene towards the ephedrine – A frequently used molecule in sport. <i>Computational and Theoretical Chemistry</i> , 2018, 1124, 39-50.	2.5	12
90	Understanding how yttrium doping influences the properties of nickel ferrite – Combined experimental and computational study. <i>Ceramics International</i> , 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. <i>Journal of the Serbian Chemical Society</i> , 2018, 83, 1-18.	0.8	12
92	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1147, 266-280.	3.6	11
95	Structural and spectroscopic characterization, reactivity study and charge transfer analysis of the newly synthesized 2-(6-hydroxy-1-benzofuran-3-yl) acetic acid. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2018, 1164, 525-538.	3.6	11
97	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. <i>Journal of Molecular Structure</i> , 2017, 1137, 589-605.	3.6	10
98	Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1H-benzimidazole.3H <sub>2</sub> O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies. <i>Journal of Molecular Structure</i> , 2017, 1149, 602-612.	3.6	10
99	Two novel imidazole derivatives – Combined experimental and computational study. <i>Journal of Molecular Structure</i> , 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. <i>Inorganica Chimica Acta</i> , 2019, 486, 698-703.	2.4	10
101	Understanding reactivity of a triazole derivative and its interaction with graphene and doped/undoped-coronene – a DFT study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2316-2326.	3.5	10
102	Investigation of reactive properties of an antiviral azatricyclo derivative – KDFIT, MD and docking simulations. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-10.	3.5	10
104	The role of environmental waters ionic composition and UV – LED radiation on photodegradation, mineralization and toxicity of commonly used UV-blockers. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 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, in vitro anticancer activity and theoretical studies. <i>Journal of Molecular Structure</i> , 2020, 1217, 128445.	3.6	9
107	Tumoricidal Potential of Novel Amino-1,10-phenanthroline Derived Imine Ligands: Chemical Preparation, Structure, and Biological Investigations. <i>Molecules</i> , 2020, 25, 2865.	3.8	9
108	Optoelectronic properties of higher acenes, their BN analogue and substituted derivatives. <i>Materials Chemistry and Physics</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1127, 427-436.	3.6	8
110	Complexes of Zn(II) and Cd(II) with 2-acetylpyridine -aminoguanidine " Syntheses, structures and DFT calculations. <i>Inorganica Chimica Acta</i> , 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. <i>Journal of Molecular Structure</i> , 2021, 1230, 129898.	3.6	8
112	PbSe sensitized with iodine and oxygen: a combined computational and experimental study. <i>Journal of Alloys and Compounds</i> , 2021, , 163119.	5.5	8
113	Optical properties of layers of symmetric molecular nanofilms. <i>Journal of Optics (India)</i> , 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. <i>Polyhedron</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1150, 358-365.	3.6	7
116	SURFACE LOCALIZATION OF ELECTRONS IN ULTRATHIN CRYSTALLINE STRUCTURES. <i>Modern Physics Letters B</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1135, 234-246.	3.6	6
119	Structural, biological and in-silico study of quinoline-based chalcogensemicarbazones. <i>Journal of Molecular Structure</i> , 2020, 1203, 127482.	3.6	6
120	Linking azoles to isoniazid via hydrazone bridge: Synthesis, crystal structure determination, antitubercular evaluation and computational studies. <i>Journal of Molecular Liquids</i> , 2022, 354, 118873.	4.9	6
121	Investigation of reactive and spectroscopic properties of oxobutanoic acid derivative: Combined spectroscopic, DFT, MD and docking study. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Liquids</i> , 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. <i>Journal of Molecular Structure</i> , 2017, 1147, 121-128.	3.6	3
124	Unprecedented copper(ii) coordination induced nucleophilic cleavage of a quinoxaline heterocycle: structural and computational studies. <i>CrystEngComm</i> , 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. <i>Nanomaterials</i> , 2022, 12, 1901.	4.1	3
126	Modeling of fundamental electronic circuits by the Euler method using the Python programming language. <i>Physics Education</i> , 2020, 55, 055016.	0.5	2



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127	Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. <i>Symmetry</i> , 2021, 13, 1619.	2.2	2
128	Removal of hydrochlorothiazide from drinking and environmental water: Hydrolysis, direct and indirect photolysis. <i>Energy and Environment</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Journal of Molecular Structure</i> , 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. <i>Proceedings (mdpi)</i> , 2019, 15, 28.	0.2	0
133	Particularities in physical characteristics of molecular crystalline nanofilms. <i>Zbornik Matice Srpske Za Prirodne Nauke</i> , 2010, , 115-125.	0.1	0
134	Structural and computational study of quinoline-based chalcogensemicarbazones. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, e566-e566.	0.1	0