Stevan Armakovic

List of Publications by Citations

132 papers	2,284 citations	29 h-index	38 g-index
140 ext. papers	2,707 ext. citations	3.6 avg, IF	5.45 L-index

#	Paper	IF	Citations
132	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	3.7	86
131	Quinoline derivatives as possible lead compounds for anti-malarial drugs: Spectroscopic, DFT and MD study. *Arabian Journal of Chemistry*, **2020**, 13, 632-648	5.9	71
130	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	3.4	70
129	Active components of frequently used Eblockers from the aspect of computational study. *Journal of Molecular Modeling*, **2012**, 18, 4491-501	2	54
128	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	4.4	53
127	Understanding reactivity of two newly synthetized imidazole derivatives by spectroscopic characterization and computational study. *Journal of Molecular Structure*, **2018**, 1158, 176-196	3.4	49
126	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, 530-533	3.4	46
125	Optoelectronic properties of curved carbon systems. *Carbon*, **2017**, 111, 371-379	10.4	44
124	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	3.4	44
123	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	3.4	44
122	Efficiency of La-doped TiO2 calcined at different temperatures in photocatalytic degradation of Eblockers. *Arabian Journal of Chemistry*, **2019**, 12, 5355-5369	5.9	44
121	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	3.4	41
120	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, 111997-112013	3.7	38
119	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	3.4	38
118	Theoretical investigation of loratadine reactivity in order to understand its degradation properties: DFT and MD study. *Journal of Molecular Modeling*, **2016**, 22, 240	2	37
117	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	2.5	37
116	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	1.3	37

115	Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures. *Journal of Molecular Structure*, **2017**, 1141, 495-511	3.4	36
114	Sumanene and its adsorption properties towards CO, CO₂ and NH₃ molecules. *Journal of Molecular Modeling*, **2014**, 20, 2170	2	36
113	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	3.4	35
112	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	4.4	35
111	Influence of sumanene modifications with boron and nitrogen atoms to its hydrogen adsorption properties. *Physical Chemistry Chemical Physics*, **2016**, 18, 2859-70	3.6	32
110	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	3.4	32
109	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	3.4	32
108	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	4.4	31
107	Hydrogen storage properties of sumanene. *International Journal of Hydrogen Energy*, **2013**, 38, 12190-12198	3.7	31
106	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	3.4	29
105	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	3.4	29
104	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. *Journal of Molecular Structure*, **2020**, 1205, 127587	3.4	29
103	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	3.4	27
102	Synthesis, characterization and computational studies of semicarbazide derivative. *Journal of Molecular Liquids*, **2018**, 272, 481-495	6	27
101	Structuring of water in the new generation ionic liquid □Comparative experimental and theoretical study. *Journal of Chemical Thermodynamics*, **2016**, 93, 164-171	2.9	26
100	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	3.4	25
99	Aromaticity, response, and nonlinear optical properties of sumanene modified with boron and nitrogen atoms. *Journal of Molecular Modeling*, **2014**, 20, 2538	2	25
98	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	3.4	25

97	A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene – A frequently used benzene derivative. *Journal of Molecular Structure*, **2018**, 1151, 245-255	3.4	24
96	Synthesis, characterization and computational study of the newly synthetized sulfonamide molecule. *Journal of Molecular Structure*, **2018**, 1153, 212-229	3.4	22
95	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	3.4	22
94	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	6	22
93	Structure making properties of 1-(2-hydroxylethyl)-3-methylimidazolium chloride ionic liquid. *Journal of Chemical Thermodynamics*, **2016**, 95, 174-179	2.9	20
92	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	3.4	20
91	Self-assembling, reactivity and molecular dynamics of fullerenol nanoparticles. *Physical Chemistry Chemical Physics*, **2016**, 19, 135-144	3.6	19
90	Interactions of Schiff base compounds and their coordination complexes with the drug cisplatin. *New Journal of Chemistry*, **2018**, 42, 5834-5843	3.6	19
89	Specificities of boron disubstituted sumanenes. *Journal of Molecular Modeling*, **2013**, 19, 1153-66	2	19
88	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	9.3	19
87	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	3.6	19
86	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	4.4	18
85	Determination of reactive properties of 1-butyl-3-methylimidazolium taurate ionic liquid employing DFT calculations. *Journal of Molecular Liquids*, **2016**, 222, 796-803	6	18
84	Remarkable colorimetric sensing behavior of pyrazole-based chemosensor towards Cu(ii) ion detection: synthesis, characterization and theoretical investigations.. *RSC Advances*, **2018**, 8, 18023-18029	3.7	18
83	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	3.4	17
82	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). *Journal of Molecular Structure*, **2019**, 1195, 815-826	3.4	17
81	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	3.4	17
80	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	3.4	17

79	Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of N?-diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide. *Journal of Molecular Structure*, **2017**, 1130, 208-222	3.4	17
78	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. *Journal of Molecular Structure*, **2018**, 1155, 184-195	3.4	16
77	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	3.4	16
76	Kosmotropism of newly synthesized 1-butyl-3-methylimidazolium taurate ionic liquid: Experimental and computational study. *Journal of Chemical Thermodynamics*, **2016**, 94, 85-95	2.9	15
75	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	3.4	14
74	Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione. *Journal of Molecular Structure*, **2019**, 1175, 269-279	3.4	14
73	Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative. *Journal of Molecular Structure*, **2019**, 1176, 881-894	3.4	14
72	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. *Journal of Molecular Structure*, **2017**, 1135, 1-14	3.4	13
71	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	3.4	13
70	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	3.4	13
69	Fullerene C as a potential carrier of ephedrine drug - a computational study of interactions and influence of temperature. *Physical Chemistry Chemical Physics*, **2019**, 21, 23329-23337	3.6	13
68	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	3.4	13
67	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. *Journal of Molecular Structure*, **2017**, 1134, 25-39	3.4	12
66	DFT study of 1-butyl-3-methylimidazolium salicylate: a third-generation ionic liquid. *Journal of Molecular Modeling*, **2015**, 21, 246	2	12
65	Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxymethyl benzimidazole. *Journal of Molecular Structure*, **2017**, 1129, 86-97	3.4	12
64	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	3.4	12
63	Coordination compounds of a hydrazone derivative with Co(III), Ni(II), Cu(II) and Zn(II): synthesis, characterization, reactivity assessment and biological evaluation. *New Journal of Chemistry*, **2016**, 40, 5885-5895	3.6	12
62	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	3.4	11

61	Optoelectronic and charge carrier hopping properties of ultra-thin boron nitride nanotubes. *Superlattices and Microstructures*, **2015**, 79, 79-85	2.8	11
60	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	3.4	11
59	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	3.4	11
58	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. *Journal of Molecular Structure*, **2017**, 1134, 814-827	3.4	10
57	Design, synthesis and computational analysis of novel acridine-(sulfadiazine/sulfathiazole) hybrids as antibacterial agents. *Journal of Molecular Structure*, **2019**, 1186, 39-49	3.4	10
56	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	0.9	10
55	Experimental and computational study of hydrolysis and photolysis of antibiotic ceftriaxone: Degradation kinetics, pathways, and toxicity. *Science of the Total Environment*, **2021**, 768, 144991	10.2	10
54	Two novel imidazole derivatives – Combined experimental and computational study. *Journal of Molecular Structure*, **2018**, 1173, 221-239	3.4	10
53	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. *Journal of Molecular Structure*, **2017**, 1137, 589-605	3.4	9
52	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	3.4	9
51	Investigation of 1,2,3-trialkylimidazolium ionic liquids: experiment and density functional theory calculations. *New Journal of Chemistry*, **2017**, 41, 650-660	3.6	9
50	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	12.8	9
49	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	6	9
48	A DFT and MD study of reactive, H2 adsorption and optoelectronic properties of graphane nanoparticles – An influence of boron doping. *Materials Chemistry and Physics*, **2020**, 241, 122329	4.4	9
47	Pyridoxylidene aminoguanidine and its copper(II) complexes – Syntheses, structure, and DFT calculations. *Journal of Coordination Chemistry*, **2017**, 70, 2870-2887	1.6	8
46	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	3.4	8
45	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	3.4	7
44	Electronic structure of yttrium-doped zinc ferrite – Insights from experiment and theory. *Journal of Alloys and Compounds*, **2020**, 842, 155704	5.7	7

43	Adsorption properties of graphene towards the ephedrine A frequently used molecule in sport. *Computational and Theoretical Chemistry*, **2018**, 1124, 39-50	2	7
42	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	3.9	7
41	Optoelectronic properties of higher acenes, their BN analogue and substituted derivatives. *Materials Chemistry and Physics*, **2016**, 170, 210-217	4.4	7
40	Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1 H -benzoimidazole.3H 2 O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies. *Journal of Molecular Structure*, **2017**, 1149, 602-612	3.4	7
39	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	3.4	7
38	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	2.7	7
37	Uncommon structure making/breaking behaviour of cholinium taurate in water. *Journal of Chemical Thermodynamics*, **2017**, 107, 58-64	2.9	6
36	Understanding how yttrium doping influences the properties of nickel ferrite Combined experimental and computational study. *Ceramics International*, **2019**, 45, 20290-20296	5.1	6
35	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	3.4	6
34	Optical properties of layers of symmetric molecular nanofilms. *Journal of Optics (India)*, **2015**, 44, 1-6	1.3	6
33	Reactivity properties and adsorption behavior of a triazole derivative DFT and MD simulation studies. *Journal of Molecular Liquids*, **2021**, 341, 117439	6	6
32	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	3.4	5
31	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	3.4	5
30	Complexes of Zn(II) and Cd(II) with 2-acetylpyridine -aminoguanidine Syntheses, structures and DFT calculations. *Inorganica Chimica Acta*, **2018**, 473, 160-168	2.7	5
29	Structural, biological and in-silico study of quinoline-based chalcogensemicarbazones. *Journal of Molecular Structure*, **2020**, 1203, 127482	3.4	5
28	Understanding reactivity of a triazole derivative and its interaction with graphene and doped/undoped-coronene-a DFT study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-11	3.6	5
27	Investigation of the reactivity properties of a thiourea derivative with anticancer activity by DFT and MD simulations. *Journal of Molecular Modeling*, **2021**, 27, 217	2	5
26	Structural, antioxidant, antiproliferative and in-silico study of pyridine-based hydrazonyl-selenazoles and their sulphur isosteres. *Journal of Molecular Structure*, **2021**, 1240, 130512	3.4	5

25	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	2.7	4
24	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. *Journal of Molecular Structure*, **2020**, 1217, 128445	3.4	4
23	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	3.4	4
22	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	4
21	Biomass waste utilization for adsorbent preparation in CO2 capture and sustainable environment applications. *Sustainable Energy Technologies and Assessments*, **2021**, 46, 101288	4.7	4
20	Sumanene as a delivery system for 5-fluorouracil drug DFT, SAPT and MD study. *Journal of Molecular Liquids*, **2021**, 342, 117526	6	4
19	SURFACE LOCALIZATION OF ELECTRONS IN ULTRATHIN CRYSTALLINE STRUCTURES. *Modern Physics Letters B*, **2014**, 28, 1450023	1.6	3
18	Investigation of reactive properties of an antiviral azatricyclo derivative DFT, MD and docking simulations. *Journal of Molecular Structure*, **2021**, 1230, 129937	3.4	3
17	Tumoricidal Potential of Novel Amino-1,10-phenanthroline Derived Imine Ligands: Chemical Preparation, Structure, and Biological Investigations. *Molecules*, **2020**, 25,	4.8	2
16	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	3.4	2
15	PbSe sensitized with iodine and oxygen: a combined computational and experimental study. *Journal of Alloys and Compounds*, **2021**, 163119	5.7	2
14	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	3.6	2
13	The role of environmental waters ionic composition and UV ED radiation on photodegradation, mineralization and toxicity of commonly used blockers. *Journal of Molecular Structure*, **2021**, 1249, 131579	3.4	2
12	Modeling of fundamental electronic circuits by the Euler method using the Python programming language. *Physics Education*, **2020**, 55, 055016	0.8	1
11	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	3.4	1
10	Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. *Symmetry*, **2021**, 13, 1619	2.7	1
9	Unprecedented copper(II) coordination induced nucleophilic cleavage of a quinoxaline heterocycle: structural and computational studies. *CrystEngComm*, **2021**, 23, 5078-5086	3.3	1
8	Linking azoles to isoniazid via hydrazone bridge: Synthesis, crystal structure determination, antitubercular evaluation and computational studies. *Journal of Molecular Liquids*, **2022**, 354, 118873	6	1

7	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	6	0
6	Removal of hydrochlorothiazide from drinking and environmental water: Hydrolysis, direct and indirect photolysis. *Energy and Environment*,0958305X2210840	2.4	0
5	Comprehensive Study of the Chemistry behind the Stability of Carboxylic SWCNT Dispersions in the Development of a Transparent Electrode. *Nanomaterials*, **2022**, 12, 1901	5.4	0
4	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	3.4	
3	Potential of Sumanene Modified with Boron and Nitrogen Atoms for Adsorption of Carbon Dioxide: DFT and SAPT Study. *Proceedings (mdpi)*, **2019**, 15, 28	0.3	
2	Particularities in physical characteristics of molecular crystalline nanofilms. *Zbornik Matice Srpske Za Prirodne Nauke*, **2010**, 115-125	0.3	
1	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**, 133315	3.4	