

Sanja J Armakovic

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130
papers

2,581
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30
h-index

42
g-index

138
ext. papers

3,011
ext. citations

3.8
avg, IF

5.44
L-index

#	Paper	IF	Citations
130	Photocatalytic degradation of metoprolol tartrate in suspensions of two TiO ₂ -based photocatalysts with different surface area. Identification of intermediates and proposal of degradation pathways. <i>Journal of Hazardous Materials</i> , 2011 , 198, 123-32	12.8	95
129	Influence of electron acceptors on the kinetics of metoprolol photocatalytic degradation in TiO ₂ suspension. A combined experimental and theoretical study. <i>RSC Advances</i> , 2015 , 5, 54589-54604	3.7	86
128	Degradation of thiamethoxam and metoprolol by UV, O ₃ and UV/O ₃ hybrid processes: Kinetics, degradation intermediates and toxicity. <i>Journal of Hydrology</i> , 2012 , 472-473, 314-327	6	82
127	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	5.9	71
126	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	3.4	70
125	Active components of frequently used β -blockers from the aspect of computational study. <i>Journal of Molecular Modeling</i> , 2012 , 18, 4491-501	2	54
124	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	4.4	53
123	Understanding reactivity of two newly synthesized imidazole derivatives by spectroscopic characterization and computational study. <i>Journal of Molecular Structure</i> , 2018 , 1158, 176-196	3.4	49
122	Synthesis, XRD crystal structure, spectroscopic characterization (FT-IR, ¹ H and ¹³ 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. <i>Journal of Molecular Structure</i> , 2019 , 1177, 47-54	3.4	46
121	Toxicity assessment of metoprolol and its photodegradation mixtures obtained by using different type of TiO ₂ catalysts in the mammalian cell lines. <i>Science of the Total Environment</i> , 2013 , 463-464, 968-74	10.2	45
120	Optoelectronic properties of curved carbon systems. <i>Carbon</i> , 2017 , 111, 371-379	10.4	44
119	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	3.4	44
118	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	3.4	44
117	Efficiency of La-doped TiO ₂ calcined at different temperatures in photocatalytic degradation of β -blockers. <i>Arabian Journal of Chemistry</i> , 2019 , 12, 5355-5369	5.9	44
116	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	3.4	41
115	Surface modification of sol-gel synthesized TiO ₂ nanoparticles induced by La-doping. <i>Materials Characterization</i> , 2014 , 88, 30-41	3.9	39
114	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, 111997-112013	3.7	38

113	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	3.4	38
112	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	2	37
111	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	2.5	37
110	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	1.3	37
109	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	3.4	36
108	Sumanene and its adsorption properties towards CO, CO ₂ and NH ₃ molecules. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2170	2	36
107	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. <i>Journal of Molecular Structure</i> , 2017 , 1129, 72-85	3.4	35
106	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	4.4	35
105	Influence of sumanene modifications with boron and nitrogen atoms to its hydrogen adsorption properties. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 2859-70	3.6	32
104	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	3.4	32
103	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	4.4	31
102	Hydrogen storage properties of sumanene. <i>International Journal of Hydrogen Energy</i> , 2013 , 38, 12190-12198	2.9	31
101	Photocatalytic degradation of metoprolol in water suspension of TiO ₂ nanopowders prepared using sol-gel route. <i>Journal of Sol-Gel Science and Technology</i> , 2012 , 61, 390-402	2.3	30
100	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	3.4	29
99	Improved efficiency of sol-gel synthesized mesoporous anatase nanopowders in photocatalytic degradation of metoprolol. <i>Materials Research Bulletin</i> , 2013 , 48, 1363-1371	5.1	29
98	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	3.4	29
97	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. <i>Journal of Molecular Structure</i> , 2020 , 1205, 127587	3.4	29
96	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	3.4	27

95	Synthesis, characterization and computational studies of semicarbazide derivative. <i>Journal of Molecular Liquids</i> , 2018 , 272, 481-495	6	27
94	Structuring of water in the new generation ionic liquid [Comparative experimental and theoretical study. <i>Journal of Chemical Thermodynamics</i> , 2016 , 93, 164-171	2.9	26
93	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	3.4	25
92	Aromaticity, response, and nonlinear optical properties of sumanene modified with boron and nitrogen atoms. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2538	2	25
91	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	3.4	25
90	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	3.4	24
89	Photocatalytic decomposition of selected biologically active compounds in environmental waters using TiO ₂ /polyaniline nanocomposites: Kinetics, toxicity and intermediates assessment. <i>Environmental Pollution</i> , 2018 , 239, 457-465	9.3	22
88	Synthesis, characterization and computational study of the newly synthesized sulfonamide molecule. <i>Journal of Molecular Structure</i> , 2018 , 1153, 212-229	3.4	22
87	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	3.4	22
86	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	6	22
85	Structure making properties of 1-(2-hydroxyethyl)-3-methylimidazolium chloride ionic liquid. <i>Journal of Chemical Thermodynamics</i> , 2016 , 95, 174-179	2.9	20
84	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	3.4	20
83	Self-assembling, reactivity and molecular dynamics of fullerene nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2016 , 19, 135-144	3.6	19
82	Interactions of Schiff base compounds and their coordination complexes with the drug cisplatin. <i>New Journal of Chemistry</i> , 2018 , 42, 5834-5843	3.6	19
81	Specificities of boron disubstituted sumanenes. <i>Journal of Molecular Modeling</i> , 2013 , 19, 1153-66	2	19
80	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	9.3	19
79	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	3.6	19
78	Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuon. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 228, 117580	4.4	18

77	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	6	18
76	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	3.7	18
75	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	3.4	17
74	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	3.4	17
73	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	3.4	17
72	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	3.4	17
71	Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of N?-diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide. <i>Journal of Molecular Structure</i> , 2017 , 1130, 208-222	3.4	17
70	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. <i>Journal of Molecular Structure</i> , 2018 , 1155, 184-195	3.4	16
69	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	3.4	16
68	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	2.9	15
67	Photocatalytic Degradation of Herbicide Quinmerac in Various Types of Natural Water. <i>Water, Air, and Soil Pollution</i> , 2012 , 223, 3009-3020	2.6	15
66	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	3.4	14
65	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	3.4	14
64	Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative. <i>Journal of Molecular Structure</i> , 2019 , 1176, 881-894	3.4	14
63	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. <i>Journal of Molecular Structure</i> , 2017 , 1135, 1-14	3.4	13
62	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	3.4	13
61	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	3.4	13
60	Fullerene C 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	3.6	13

59	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	3.4	13
58	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	3.4	12
57	DFT study of 1-butyl-3-methylimidazolium salicylate: a third-generation ionic liquid. <i>Journal of Molecular Modeling</i> , 2015 , 21, 246	2	12
56	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	3.4	12
55	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	3.4	12
54	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	3.6	12
53	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	3.4	11
52	Optoelectronic and charge carrier hopping properties of ultra-thin boron nitride nanotubes. <i>Superlattices and Microstructures</i> , 2015 , 79, 79-85	2.8	11
51	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	3.4	11
50	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	3.4	11
49	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. <i>Journal of Molecular Structure</i> , 2017 , 1134, 814-827	3.4	10
48	Design, synthesis and computational analysis of novel acridine-(sulfadiazine/sulfathiazole) hybrids as antibacterial agents. <i>Journal of Molecular Structure</i> , 2019 , 1186, 39-49	3.4	10
47	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	0.9	10
46	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	10.2	10
45	Two novel imidazole derivatives [Combined experimental and computational study. <i>Journal of Molecular Structure</i> , 2018 , 1173, 221-239	3.4	10
44	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. <i>Journal of Molecular Structure</i> , 2017 , 1137, 589-605	3.4	9
43	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	3.4	9
42	Investigation of 1,2,3-trialkylimidazolium ionic liquids: experiment and density functional theory calculations. <i>New Journal of Chemistry</i> , 2017 , 41, 650-660	3.6	9

41	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	12.8	9
40	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	6	9
39	A DFT and MD study of reactive, H ₂ adsorption and optoelectronic properties of graphane nanoparticles [An influence of boron doping. <i>Materials Chemistry and Physics</i> , 2020 , 241, 122329	4.4	9
38	Pyridoxylidene aminoguanidine and its copper(II) complexes [Syntheses, structure, and DFT calculations. <i>Journal of Coordination Chemistry</i> , 2017 , 70, 2870-2887	1.6	8
37	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	3.4	8
36	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	3.4	7
35	Adsorption properties of graphene towards the ephedrine [A frequently used molecule in sport. <i>Computational and Theoretical Chemistry</i> , 2018 , 1124, 39-50	2	7
34	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	3.9	7
33	Optoelectronic properties of higher acenes, their BN analogue and substituted derivatives. <i>Materials Chemistry and Physics</i> , 2016 , 170, 210-217	4.4	7
32	Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1 H -benzimidazole.3H 2 O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies. <i>Journal of Molecular Structure</i> , 2017 , 1149, 602-612	3.4	7
31	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	3.4	7
30	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	2.7	7
29	Uncommon structure making/breaking behaviour of cholinium taurate in water. <i>Journal of Chemical Thermodynamics</i> , 2017 , 107, 58-64	2.9	6
28	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	3.4	6
27	Reactivity properties and adsorption behavior of a triazole derivative [DFT and MD simulation studies. <i>Journal of Molecular Liquids</i> , 2021 , 341, 117439	6	6
26	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	3.4	5
25	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	3.4	5
24	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	2.7	5

23	Structural, biological and in-silico study of quinoline-based chalcogen semicarbazones. <i>Journal of Molecular Structure</i> , 2020 , 1203, 127482	3.4	5
22	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> , 2020 , 1-11	3.6	5
21	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	2	5
20	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	3.4	5
19	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	2.7	4
18	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	3.4	4
17	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	3.4	4
16	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	4
15	Sumanene as a delivery system for 5-fluorouracil drug DFT, SAPT and MD study. <i>Journal of Molecular Liquids</i> , 2021 , 342, 117526	6	4
14	Investigation of reactive properties of an antiviral azatricyclo derivative DFT, MD and docking simulations. <i>Journal of Molecular Structure</i> , 2021 , 1230, 129937	3.4	3
13	Tumoricidal Potential of Novel Amino-1,10-phenanthroline Derived Imine Ligands: Chemical Preparation, Structure, and Biological Investigations. <i>Molecules</i> , 2020 , 25,	4.8	2
12	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	3.4	2
11	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	3.6	2
10	The role of environmental waters ionic composition and UV-LED radiation on photodegradation, mineralization and toxicity of commonly used B-blockers. <i>Journal of Molecular Structure</i> , 2021 , 1249, 131579	3.4	2
9	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	3.4	1
8	Water-Active Titanium/Molybdenum/Mixed-Oxides: Removal Efficiency of Organic Water Pollutants by Adsorption and Photocatalysis and Toxicity Assessment. <i>Catalysts</i> , 2021 , 11, 1054	4	1
7	Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. <i>Symmetry</i> , 2021 , 13, 1619	2.7	1
6	Unprecedented copper(II) coordination induced nucleophilic cleavage of a quinoxaline heterocycle: structural and computational studies. <i>CrystEngComm</i> , 2021 , 23, 5078-5086	3.3	1

5	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	6	1
4	Removal of hydrochlorothiazide from drinking and environmental water: Hydrolysis, direct and indirect photolysis. <i>Energy and Environment</i> , 0958305X2210840	2.4	0
3	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	3.4	
2	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	0.3	
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. <i>Journal of Molecular Structure</i> , 2022 , 133315	3.4	