

Sanja J Armakovic

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

130
papers

2,581
citations

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	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
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 , 133315	3.4	
128	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
127	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
126	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
125	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
124	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
123	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
122	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
121	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
120	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
119	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
118	Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. <i>Symmetry</i> , 2021 , 13, 1619	2.7	1
117	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
116	The role of environmental waters ionic composition and UV-LED radiation on photodegradation, mineralization and toxicity of commonly used blockers. <i>Journal of Molecular Structure</i> , 2021 , 1249, 131579	3.4	2
115	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
114	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

113	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
112	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
111	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
110	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
109	Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuiron. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020 , 228, 117580	4.4	18
108	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
107	Structural, biological and in-silico study of quinoline-based chalcogensemicarbazones. <i>Journal of Molecular Structure</i> , 2020 , 1203, 127482	3.4	5
106	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
105	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
104	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
103	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
102	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
101	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
100	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
99	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
98	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
97	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	
96	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

95	Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative. <i>Journal of Molecular Structure</i> , 2019 , 1176, 881-894	3-4	14
94	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
93	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
92	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
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	Efficiency of La-doped TiO ₂ calcined at different temperatures in photocatalytic degradation of Eblockers. <i>Arabian Journal of Chemistry</i> , 2019 , 12, 5355-5369	5-9	44
89	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
88	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
87	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
86	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
85	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
84	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
83	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
82	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
81	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
80	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
79	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
78	Synthesis, characterization and computational study of the newly synthesized sulfonamide molecule. <i>Journal of Molecular Structure</i> , 2018 , 1153, 212-229	3-4	22

77	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
76	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
75	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
74	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
73	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
72	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
71	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
70	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
69	Synthesis, characterization and computational studies of semicarbazide derivative. <i>Journal of Molecular Liquids</i> , 2018 , 272, 481-495	6	27
68	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
67	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	2.7	18
66	Two novel imidazole derivatives [Combined experimental and computational study. <i>Journal of Molecular Structure</i> , 2018 , 1173, 221-239	3.4	10
65	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
64	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
63	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
62	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
61	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
60	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

59	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. <i>Journal of Molecular Structure</i> , 2017 , 1137, 589-605	3-4	9
58	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, 118-123	3-4	9
57	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
56	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
55	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	
54	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
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	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
51	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
50	Uncommon structure making/breaking behaviour of cholinium taurate in water. <i>Journal of Chemical Thermodynamics</i> , 2017 , 107, 58-64	2-9	6
49	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
48	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
47	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
46	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
45	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
44	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
43	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
42	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. <i>Journal of Molecular Structure</i> , 2017 , 1149, 602-612	3-4	7

41	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
40	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
39	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
38	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
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	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
35	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
34	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
33	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
32	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
31	Optoelectronic properties of curved carbon systems. <i>Carbon</i> , 2017 , 111, 371-379	10.4	44
30	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. <i>Journal of Molecular Structure</i> , 2017 , 1128, 694-706	3.4	46
29	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
28	Self-assembling, reactivity and molecular dynamics of fullerene nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2016 , 19, 135-144	3.6	19
27	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
26	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
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	3.7	38
24	Optoelectronic properties of higher acenes, their BN analogue and substituted derivatives. <i>Materials Chemistry and Physics</i> , 2016 , 170, 210-217	4.4	7

23	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
22	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
21	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
20	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
19	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
18	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
17	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
16	DFT study of 1-butyl-3-methylimidazolium salicylate: a third-generation ionic liquid. <i>Journal of Molecular Modeling</i> , 2015 , 21, 246	2	12
15	Optoelectronic and charge carrier hopping properties of ultra-thin boron nitride nanotubes. <i>Superlattices and Microstructures</i> , 2015 , 79, 79-85	2.8	11
14	Surface modification of sol-gel synthesized TiO ₂ nanoparticles induced by La-doping. <i>Materials Characterization</i> , 2014 , 88, 30-41	3.9	39
13	Sumanene and its adsorption properties towards CO, CO ₂ and NH ₃ molecules. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2170	2	36
12	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
11	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
10	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
9	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
8	Specificities of boron disubstituted sumanenes. <i>Journal of Molecular Modeling</i> , 2013 , 19, 1153-66	2	19
7	Hydrogen storage properties of sumanene. <i>International Journal of Hydrogen Energy</i> , 2013 , 38, 12190-12198	1.98	31
6	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

5	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
4	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
3	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
2	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
1	Removal of hydrochlorothiazide from drinking and environmental water: Hydrolysis, direct and indirect photolysis. <i>Energy and Environment</i> , 0958305X2210840	2.4	0