

# Sanja J ArmakoviÄ

## List of Publications by Year in descending order

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131  
papers

3,634  
citations

108046

37  
h-index

232693

48  
g-index

138  
all docs

138  
docs citations

138  
times ranked

2438  
citing authors

#	ARTICLE	IF	CITATIONS
1	Understanding reactivity of a triazole derivative and its interaction with graphene and doped/undoped-coroneneâ€”a DFT study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2316-2326.	2.0	10
2	The role of environmental waters ionic composition and UVâ€”LED radiation on photodegradation, mineralization and toxicity of commonly used Î²-blockers. <i>Journal of Molecular Structure</i> , 2022, 1249, 131579.	1.8	10
3	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.	2.3	6
4	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.	1.8	2
5	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.	1.4	44
6	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.	1.1	20
7	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.	1.8	8
8	Investigation of reactive properties of an antiviral azatricyclo derivativeâ€”DFT, MD and docking simulations. <i>Journal of Molecular Structure</i> , 2021, 1230, 129937.	1.8	10
9	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.	3.9	23
10	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.	2.3	40
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.	2.0	10
12	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.	0.8	21
13	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.	2.3	53
14	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.	1.6	7
15	Investigation of Pharmaceutical Importance of 2H-Pyran-2-One Analogues via Computational Approaches. <i>Symmetry</i> , 2021, 13, 1619.	1.1	2
16	Structural, antioxidant, antiproliferative and inâ€”silico study of pyridine-based hydrazoneylâ€”selenazoles and their sulphur isosteres. <i>Journal of Molecular Structure</i> , 2021, 1240, 130512.	1.8	18
17	Reactivity properties and adsorption behavior of a triazole derivative â€” DFT and MD simulation studies. <i>Journal of Molecular Liquids</i> , 2021, 341, 117439.	2.3	16
18	Sumanene as a delivery system for 5-fluorouracil drug â€” DFT, SAPT and MD study. <i>Journal of Molecular Liquids</i> , 2021, 342, 117526.	2.3	20

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19	Unprecedented copper(ii) coordination induced nucleophilic cleavage of a quinoxaline heterocycle: structural and computational studies. <i>CrystEngComm</i> , 2021, 23, 5078-5086.	1.3	3
20	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.	2.3	97
21	A DFT and MD study of reactive, H <sub>2</sub> adsorption and optoelectronic properties of graphane nanoparticles " An influence of boron doping. <i>Materials Chemistry and Physics</i> , 2020, 241, 122329.	2.0	15
22	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.	2.0	69
23	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.	2.0	26
24	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. <i>Journal of Molecular Structure</i> , 2020, 1205, 127587.	1.8	53
25	Structural, biological and in-silico study of quinoline-based chalcogensemicarbazones. <i>Journal of Molecular Structure</i> , 2020, 1203, 127482.	1.8	6
26	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.	1.8	9
27	Tumoricidal Potential of Novel Amino-1,10-phenanthroline Derived Imine Ligands: Chemical Preparation, Structure, and Biological Investigations. <i>Molecules</i> , 2020, 25, 2865.	1.7	9
28	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.	6.5	14
29	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.	1.8	16
30	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
31	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.	1.8	26
32	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.	2.0	80
33	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.	1.8	27
34	Design, synthesis and computational analysis of novel acridine-(sulfadiazine/sulfathiazole) hybrids as antibacterial agents. <i>Journal of Molecular Structure</i> , 2019, 1186, 39-49.	1.8	14
35	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.	1.3	26
36	Spectroscopic, antimicrobial and computational study of novel benzoxazole derivative. <i>Journal of Molecular Structure</i> , 2019, 1176, 881-894.	1.8	17

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37	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.	1.8	71
38	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.	1.2	10
39	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.	1.8	59
40	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.	1.8	43
41	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.	2.3	54
42	Structural and computational study of quinoline-based chalcogensemicarbazones. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2019, 75, e566-e566.	0.0	0
43	Interactions of Schiff base compounds and their coordination complexes with the drug cisplatin. <i>New Journal of Chemistry</i> , 2018, 42, 5834-5843.	1.4	22
44	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.	1.8	11
45	Photocatalytic decomposition of selected biologically active compounds in environmental waters using TiO <sub>2</sub> /polyaniline nanocomposites: Kinetics, toxicity and intermediates assessment. <i>Environmental Pollution</i> , 2018, 239, 457-465.	3.7	35
46	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.	1.8	49
47	Understanding reactivity of two newly synthesized imidazole derivatives by spectroscopic characterization and computational study. <i>Journal of Molecular Structure</i> , 2018, 1158, 176-196.	1.8	56
48	Adsorption properties of graphene towards the ephedrine $\hat{a}$ €“ A frequently used molecule in sport. <i>Computational and Theoretical Chemistry</i> , 2018, 1124, 39-50.	1.1	12
49	Complexes of Zn(II) and Cd(II) with 2-acetylpyridine -aminoguanidine $\hat{a}$ €“ Syntheses, structures and DFT calculations. <i>Inorganica Chimica Acta</i> , 2018, 473, 160-168.	1.2	8
50	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.	1.8	22
51	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.	1.8	18
52	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.	1.8	11
53	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. <i>Journal of Molecular Structure</i> , 2018, 1155, 184-195.	1.8	16
54	Synthesis, characterization and computational study of the newly synthesized sulfonamide molecule. <i>Journal of Molecular Structure</i> , 2018, 1153, 212-229.	1.8	46

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55	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.	1.8	51
56	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.	1.8	19
57	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.	1.8	42
58	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.	3.7	23
59	Synthesis, characterization and computational studies of semicarbazide derivative. <i>Journal of Molecular Liquids</i> , 2018, 272, 481-495.	2.3	48
60	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.	1.1	29
61	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.	1.7	21
62	Two novel imidazole derivatives – Combined experimental and computational study. <i>Journal of Molecular Structure</i> , 2018, 1173, 221-239.	1.8	10
63	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.	2.0	45
64	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.	1.8	83
65	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.	1.8	53
66	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.	1.8	32
67	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.	0.4	12
68	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.	1.8	48
69	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.	1.8	6
70	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.	1.8	6
71	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. <i>Journal of Molecular Structure</i> , 2017, 1134, 814-827.	1.8	11
72	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. <i>Journal of Molecular Structure</i> , 2017, 1135, 1-14.	1.8	18

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73	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. <i>Journal of Molecular Structure</i> , 2017, 1137, 589-605.	1.8	10
74	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.	1.8	11
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.	1.8	20
76	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.	1.8	43
77	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.	1.8	0
78	Self-assembling, reactivity and molecular dynamics of fullerene nanoparticles. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 135-144.	1.3	25
79	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.	1.0	7
80	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.	1.8	13
81	Investigation of 1,2,3-trialkylimidazolium ionic liquids: experiment and density functional theory calculations. <i>New Journal of Chemistry</i> , 2017, 41, 650-660.	1.4	12
82	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.	1.8	20
83	Uncommon structure making/breaking behaviour of cholinium taurate in water. <i>Journal of Chemical Thermodynamics</i> , 2017, 107, 58-64.	1.0	12
84	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.	1.8	42
85	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.	1.8	9
86	Pyridoxylidene aminoguanidine and its copper(II) complexes – Syntheses, structure, and DFT calculations. <i>Journal of Coordination Chemistry</i> , 2017, 70, 2870-2887.	0.8	12
87	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.	1.8	22
88	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.	1.8	7
89	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.	1.8	18
90	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.	1.8	4



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91	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. Journal of Molecular Structure, 2017, 1149, 602-612.	1.8	10
92	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.	1.8	3
93	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.	1.8	11
94	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.	1.8	14
95	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.	1.8	35
96	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.	1.8	8
97	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.	1.8	46
98	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.	1.8	26
99	Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxyethyl benzimidazole. Journal of Molecular Structure, 2017, 1129, 86-97.	1.8	15
100	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.	1.8	39
101	Vibrational spectroscopic investigations, molecular dynamic simulations and molecular docking studies of Nâ€²-diphenylmethylidene-5-methyl-1H-pyrazole-3-carbohydrazide. Journal of Molecular Structure, 2017, 1130, 208-222.	1.8	22
102	Optoelectronic properties of curved carbon systems. Carbon, 2017, 111, 371-379.	5.4	53
103	Synthesis, XRD crystal structure, spectroscopic characterization (FT-IR, 1H and 13C NMR), DFT studies, chemical reactivity and bond dissociation energy studies using molecular dynamics simulations and evaluation of antimicrobial and antioxidant activities of a novel chalcone derivative, (E)-1-(4-bromophenyl)-3-(4-iodophenyl)prop-2-en-1-one. Journal of Molecular Structure, 2017, 1128, 520-533.	1.8	53
104	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.	1.8	14
105	Coordination compounds of a hydrazone derivative with Co(<sc>iii</sc>), Ni(<sc>ii</sc>), Cu(<sc>ii</sc>) and Zn(<sc>ii</sc>): synthesis, characterization, reactivity assessment and biological evaluation. New Journal of Chemistry, 2016, 40, 5885-5895.	1.4	18
106	Determination of reactive properties of 1-butyl-3-methylimidazolium taurate ionic liquid employing DFT calculations. Journal of Molecular Liquids, 2016, 222, 796-803.	2.3	22
107	Theoretical investigation of loratadine reactivity in order to understand its degradation properties: DFT and MD study. Journal of Molecular Modeling, 2016, 22, 240.	0.8	39
108	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.	1.9	15

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109	Spectroscopic, single crystal XRD structure, DFT and molecular dynamics investigation of 1-(3-chloro-4-fluorophenyl)-3-[3-(trifluoromethyl)phenyl]thiourea. RSC Advances, 2016, 6, 111997-112015.	1.7	46
110	Optoelectronic properties of higher acenes, their BN analogue and substituted derivatives. Materials Chemistry and Physics, 2016, 170, 210-217.	2.0	8
111	Influence of sumanene modifications with boron and nitrogen atoms to its hydrogen adsorption properties. Physical Chemistry Chemical Physics, 2016, 18, 2859-2870.	1.3	42
112	Structure making properties of 1-(2-hydroxyethyl)-3-methylimidazolium chloride ionic liquid. Journal of Chemical Thermodynamics, 2016, 95, 174-179.	1.0	30
113	Structuring of water in the new generation ionic liquid – Comparative experimental and theoretical study. Journal of Chemical Thermodynamics, 2016, 93, 164-171.	1.0	42
114	Kosmotropism of newly synthesized 1-butyl-3-methylimidazolium taurate ionic liquid: Experimental and computational study. Journal of Chemical Thermodynamics, 2016, 94, 85-95.	1.0	16
115	Influence of electron acceptors on the kinetics of metoprolol photocatalytic degradation in TiO <sub>2</sub> suspension. A combined experimental and theoretical study. RSC Advances, 2015, 5, 54589-54604.	1.7	95
116	DFT study of 1-butyl-3-methylimidazolium salicylate: a third-generation ionic liquid. Journal of Molecular Modeling, 2015, 21, 246.	0.8	16
117	Optoelectronic and charge carrier hopping properties of ultra-thin boron nitride nanotubes. Superlattices and Microstructures, 2015, 79, 79-85.	1.4	12
118	Aromaticity, response, and nonlinear optical properties of sumanene modified with boron and nitrogen atoms. Journal of Molecular Modeling, 2014, 20, 2538.	0.8	55
119	Surface modification of sol-gel synthesized TiO <sub>2</sub> nanoparticles induced by La-doping. Materials Characterization, 2014, 88, 30-41.	1.9	46
120	Sumanene and its adsorption properties towards CO, CO <sub>2</sub> and NH <sub>3</sub> molecules. Journal of Molecular Modeling, 2014, 20, 2170.	0.8	46
121	Toxicity assessment of metoprolol and its photodegradation mixtures obtained by using different type of TiO <sub>2</sub> catalysts in the mammalian cell lines. Science of the Total Environment, 2013, 463-464, 968-974.	3.9	52
122	Improved efficiency of sol-gel synthesized mesoporous anatase nanopowders in photocatalytic degradation of metoprolol. Materials Research Bulletin, 2013, 48, 1363-1371.	2.7	29
123	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.	1.2	47
124	Specificities of boron disubstituted sumanenes. Journal of Molecular Modeling, 2013, 19, 1153-1166.	0.8	21
125	Hydrogen storage properties of sumanene. International Journal of Hydrogen Energy, 2013, 38, 12190-12198.	3.8	57
126	Degradation of thiamethoxam and metoprolol by UV, O <sub>3</sub> and UV/O <sub>3</sub> hybrid processes: Kinetics, degradation intermediates and toxicity. Journal of Hydrology, 2012, 472-473, 314-327.	2.3	95



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127	Active components of frequently used $\beta$ -blockers from the aspect of computational study. Journal of Molecular Modeling, 2012, 18, 4491-4501.	0.8	61
128	Photocatalytic Degradation of Herbicide Quinmerac in Various Types of Natural Water. Water, Air, and Soil Pollution, 2012, 223, 3009-3020.	1.1	17
129	Photocatalytic degradation of metoprolol in water suspension of TiO <sub>2</sub> nanopowders prepared using sol-gel route. Journal of Sol-Gel Science and Technology, 2012, 61, 390-402.	1.1	38
130	Photocatalytic degradation of metoprolol tartrate in suspensions of two TiO <sub>2</sub> -based photocatalysts with different surface area. Identification of intermediates and proposal of degradation pathways. Journal of Hazardous Materials, 2011, 198, 123-132.	6.5	103
131	Removal of hydrochlorothiazide from drinking and environmental water: Hydrolysis, direct and indirect photolysis. Energy and Environment, 0, , 0958305X2210840.	2.7	2