Y Sheena Mary

List of Publications by Year
in descending order

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204 papers	5,003 citations	87888 38 h-index	197818 49 g-index
211 all docs	211 docs citations	211 times ranked	1878 citing authors

#	Article	IF	Citations
1	Theoretical Insights into the Solvation, Electronic, Chemical Properties and Molecular Docking of Some Thiazole Derivatives. Polycyclic Aromatic Compounds, 2023, 43, 1546-1556.	2.6	2
2	DFT Conformational, Wavefunction Based Reactivity Analysis, Docking and MD Simulations of a Carboxamide Derivative with Potential Anticancer Activity. Polycyclic Aromatic Compounds, 2023, 43, 1590-1601.	2.6	2
3	Conformational, Reactivity Analysis, Wavefunction-Based Properties, Molecular Docking and Simulations of a Benzamide Derivative with Potential Antitumor Activity-DFT and MD Simulations. Polycyclic Aromatic Compounds, 2023, 43, 2015-2031.	2.6	3
4	Quantum Mechanical Investigation into the Adsorption Pattern of Clomipramine and Methotrimeprazine HCl with Graphene and Fullerene. Polycyclic Aromatic Compounds, 2023, 43, 2219-2232.	2.6	7
5	Spectroscopic, Solvation Effects and MD Simulation of an Adamantane-Carbohydrazide Derivative, a Potential Antiviral Agent. Polycyclic Aromatic Compounds, 2023, 43, 2056-2070.	2.6	9
6	Electronic Structure, Solvation Effects and Wave Function Based Properties of a New Triazole Based Symmetric Chromene Derivative of Apigenin. Polycyclic Aromatic Compounds, 2023, 43, 2810-2822.	2.6	1
7	A foundational theoreticalAl₁₂E₁₂(Eâ€‰=â€‰N, P) adsorption and quinolone docking study: cageâ€“quinolone pairs, optics and possible therapeutic and diagnostic applications. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3630-3646.	3.5	17
8	DFT and MD investigations of the biomolecules of phenothiazine derivatives: interactions with gold and water molecules and investigations in search of effective drug for SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4522-4533.	3.5	5
9	Spectroscopic, Docking and MD Simulation Analysis of an Adamantane Derivative with Solvation Effects in Different Solvents. Polycyclic Aromatic Compounds, 2023, 43, 4203-4215.	2.6	0
10	Understanding reactivity of a triazole derivative and its interaction with graphene and doped/undoped-coroneneâ€”a DFT study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2316-2326.	3.5	10
11	Modeling the Conformational Preference, Spectral Analysis and Other Quantum Mechanical Studies on Three Bioactive Aminobenzoate Derivatives and Their SERS Active Graphene Complexes. Polycyclic Aromatic Compounds, 2022, 42, 2076-2086.	2.6	10
12	Detailed Quantum Mechanical Studies on Three Bioactive Benzimidazole Derivatives and Their Raman Enhancement on Adsorption over Graphene Sheets. Polycyclic Aromatic Compounds, 2022, 42, 2581-2590.	2.6	19
13	Detailed Electronic Structure, Physico-Chemical Properties, Excited State Properties, Virtual Bioactivity Screening and SERS Analysis of Three Guanine Based Antiviral Drugs Valacyclovir HCl Hydrate, Acyclovir and Ganciclovir. Polycyclic Aromatic Compounds, 2022, 42, 1260-1270.	2.6	20
14	Theoretical Studies into the Spectral Characteristics, Biological Activity, and Photovoltaic Cell Efficiency of Four New Polycyclic Aromatic Chalcones. Polycyclic Aromatic Compounds, 2022, 42, 608-622.	2.6	2
15	Utilization of O/S-doped graphene nanoclusters for ultrasensitive detection of flurane derivatives-DFT investigations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5320-5327.	3.5	4
16	Spectroscopic investigations, concentration dependent SERS, and molecular docking studies of a hydroxybenzylidene derivative. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6952-6964.	3.5	8
17	DFT computational study of trihalogenated aniline derivativeâ€™s adsorption onto graphene/fullerene/fullerene-like nanocages, X₁₂Y₁₂ (Xâ€‰=â€‰Al, B, and Yâ€‰=â€‰N, P). Journal of Biomolecular Structure and Dynamics, 2022, 40, 8630-8643.		20
18	Conformational Analysis, Spectroscopic Insights, Chemical Descriptors, ELF, LOL and Molecular Docking Studies of Potential Pyrimidine Derivative with Biological Activities. Polycyclic Aromatic Compounds, 2022, 42, 5160-5170.	2.6	5

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19	Computational Study of Sorbic Acid Drug Adsorption onto Coronene/Fullerene/Fullerene-Like X12Y12 (Xâ€‰=â€‰Al, B and Yâ€‰=â€‰N, P) Nanocages: DFT and Molecular Docking Investigations. Journal of Cluster Science, 2022, 33, 1809-1819.	3.6	17
20	Adsorption of Phenothiazine Derivatives on Graphene â€“ DFT, Docking and MD Simulation. Polycyclic Aromatic Compounds, 2022, 42, 5626-5637.	2.6	6
21	Modeling the structure and reactivity landscapes of a pyrazole-ammonium ionic derivative using wavefunction-dependent characteristics and screening for potential anti-inflammatory activity. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11190-11202.	3.5	3
22	Theoretical investigation on the adsorption of melamine in Al12/B12-N12/P12 fullerene-like nanocages: a platform for ultrasensitive detection of melamine. Chemical Papers, 2022, 76, 225-238.	2.2	12
23	Evidence of cluster formation of croconic acid with Ag, Au and Cu cages, enhancement of electronic properties and Raman activity. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 264, 120233.	3.9	24
24	Theoretical model study of adsorbed antimalarial-graphene dimers: doping effects, photophysical parameters, intermolecular interactions, edge adsorption, and SERS. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13581-13592.	3.5	18
25	Adsorption of a thione bioactive derivative over different silver/gold clusters â€“ DFT investigations. Computational and Theoretical Chemistry, 2022, 1207, 113497.	2.5	18
26	Investigation of the electronic properties of solvents (water, benzene, methanol) using IEFPCM model, spectroscopic investigation with docking and MD simulations of a thiadiazole derivative with anti-tumor activities. Journal of Molecular Liquids, 2022, 348, 118061.	4.9	3
27	Adsorption properties of dacarbazine with graphene/fullerene/metal nanocages â€“ Reactivity, spectroscopic and SERS analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 268, 120677.	3.9	11
28	Adsorption behavior and solvent effects of an adamantane-triazole derivative on metal clusters â€“ DFT simulation studies. Journal of Molecular Liquids, 2022, 345, 118242.	4.9	21
29	Evidence of cluster formation of pyrrole with mixed silver metal clusters, Agx-My (xÂ=Â4,5, yÂ=Â2/1 and) Tj ETQq1 1 0.784314 rgBT /Ov	2.5	28
30	Theoretical and experimental investigation of a pyrazole derivative- solvation effects, reactivity analysis and MD simulations. Chemical Physics Letters, 2022, 793, 139469.	2.6	7
31	DFT analysis of valproic acid adsorption onto Al12/B12-N12/P12 nanocages with solvent effects. Journal of Molecular Modeling, 2022, 28, 98.	1.8	10
32	Co-crystals of ethenzamide with 2-nitrobenzoic acid - Conformational analysis, MD simulations and DFT investigations. Journal of the Indian Chemical Society, 2022, 99, 100439.	2.8	0
33	Spectroscopic analyses on an azatricycloderivative by DFT with different solvents, reactivity analysis and MD simulations. Journal of Molecular Structure, 2022, 1260, 132845.	3.6	0
34	DFT of 5-Fluoro-2-Oxo-1H-Pyrazine-3-Carboxamide (OPC) Adsorption, Spectroscopic, Solvent Effect, and SERS Analysis. Journal of Molecular Liquids, 2022, 357, 119076.	4.9	35
35	Selective detection of Fâ^' ion and SO2 molecule: An experimental and DFT study. Journal of Molecular Liquids, 2022, 359, 119329.	4.9	16
36	DFT study of 6-amino-3-(1-hydroxyethyl) pyridine-2,4-diol (AHP) adsorption on Coronene. Journal of Molecular Liquids, 2022, 360, 119436.	4.9	20

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37	Computational study of furosemide-piperazine (FS â€“ PZ) and 2,3,5,6-tetramethylpyrazine (FS-TP) co-crystals. Journal of Molecular Liquids, 2022, 360, 119537.	4.9	9
38	Adsorption of Diospyrin on the surface of CC/AlN/AlP/GaN Nanotubes: A DFT investigation. Journal of Molecular Liquids, 2022, 360, 119472.	4.9	24
39	Understanding the mechanism of thioguanine's binding to Ag6 and bimetallic (Ag3â€“Au3 and Ag3â€“Cu3) clusters. Journal of Molecular Structure, 2022, 1265, 133415.	3.6	16
40	Adsorption of a thione derivative on carbon, AlN, and BN nanotubes: a detailed DFT and MD investigation. Journal of Molecular Modeling, 2022, 28, .	1.8	12
41	Insights into solvation effects, spectroscopic, Hirshfeld surface Analysis, reactivity analysis and anti-Covid-19 ability of doxylamine succinate: Experimental, DFT, MD and docking simulations. Journal of Molecular Liquids, 2022, 361, 119609.	4.9	11
42	Synthesis, crystal structure and anti-tumour activity studies of 4-Tertiarybutylcyclohexanonethiosemicarbazone. Journal of Molecular Structure, 2022, 1265, 133490.	3.6	3
43	Sumanene as a delivery carrier for methimazole drug: DFT, AIM, SERS and solvent effects. Computational and Theoretical Chemistry, 2022, 1215, 113811.	2.5	16
44	Experimental spectra, electronic properties (liquid and gaseous phases) and activity against SARS-CoV-2 main protease of Fluphenazine dihydrochloride: DFT and MD simulations. Journal of Molecular Structure, 2022, 1267, 133633.	3.6	1
45	Quantum Mechanical Studies of Three Aromatic Halogen-Substituted Bioactive Sulfonamidobenzoxazole Compounds with Potential Light Harvesting Properties. Polycyclic Aromatic Compounds, 2021, 41, 1563-1579.	2.6	28
46	Structural study of letrozole and metronidazole and formation of self-assembly with graphene and fullerene with the enhancement of physical, chemical and biological activities. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5509-5515.	3.5	36
47	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.	2.6	44
48	DFT computational study towards investigating psychotropic drugs, promazine and trifluoperazine adsorption on graphene, fullerene and carbon cyclic ring nanoclusters. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 246, 119012.	3.9	28
49	Utilization of doped/undoped graphene quantum dots for ultrasensitive detection of duphaston, a SERS platform. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 244, 118865.	3.9	30
50	DFT, SERS-concentration and solvent dependent and docking studies of a bioactive benzenesulfonamide derivative. Journal of Molecular Structure, 2021, 1228, 129680.	3.6	23
51	Conformational analysis and quantum descriptors of two bifonazole derivatives of immense anti-tuber potential by using vibrational spectroscopy and molecular docking studies. Structural Chemistry, 2021, 32, 859-867.	2.0	9
52	Conformational analysis and DFT investigations of two triazole derivatives and its halogenated substitution by using spectroscopy, AIM and Molecular docking. Chemical Data Collections, 2021, 31, 100625.	2.3	16
53	Concentration dependent SERS, DFT and molecular docking studies of a ureido derivative with antitubercular properties. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 249, 119329.	3.9	19
54	Spectroscopic investigations, concentration dependent SERS, and molecular docking studies of a benzoic acid derivative. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 248, 119265.	3.9	20

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55	Biological perspective of a triazine derivative with isatin/chalcone/acridone: DFT and docking investigations. Structural Chemistry, 2021, 32, 19-26.	2.0	2
56	Optoelectronic properties of the newly designed 1,3,5-triazine derivatives with isatin, chalcone and acridone moieties. Computational and Theoretical Chemistry, 2021, 1197, 113160.	2.5	20
57	Adsorption of adipic acid in Al/B-N/P nanocages: DFT investigations. Journal of Molecular Modeling, 2021, 27, 113.	1.8	35
58	Spectroscopic and DFT investigations of 8-hydroxy quinoline-5-sulfonic acid-5-chloro-8-hydroxyquinoline cocrystal. Chemical Papers, 2021, 75, 3387-3399.	2.2	2
59	DFT, docking, MD simulation, and vibrational spectra with SERS analysis of a benzoxazole derivative: an anti-cancerous drug. Chemical Papers, 2021, 75, 4269-4284.	2.2	4
60	Investigation of reactive properties of an antiviral azatricyclo derivativeâ€“KDFT, MD and docking simulations. Journal of Molecular Structure, 2021, 1230, 129937.	3.6	10
61	DFT, molecular docking and SERS (concentration and solvent dependant) investigations of a methylisoxazole derivative with potential antimicrobial activity. Journal of Molecular Structure, 2021, 1232, 130034.	3.6	15
62	Theoretical investigation on the reactive and interaction properties of sorafenib â€“ DFT, AIM, spectroscopic and Hirshfeld analysis, docking and dynamics simulation. Journal of Molecular Liquids, 2021, 330, 115652.	4.9	34
63	Modeling the structural and reactivity properties of hydrazono methyl-4H-chromen-4-one derivativesâ€”wavefunction-dependent properties, molecular docking, and dynamics simulation studies. Journal of Molecular Modeling, 2021, 27, 186.	1.8	9
64	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.	4.9	40
65	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.	3.5	10
66	MD, DFT Investigations and Inhibition of the Novel SARS- CoV-2 Mainprotease in Three Cocrystals of Hydrochloro- thiazide. Analytical Chemistry Letters, 2021, 11, 450-468.	1.0	3
67	Investigation of the reactivity properties of a thiourea derivative with anticancer activity by DFT and MD simulations. Journal of Molecular Modeling, 2021, 27, 217.	1.8	21
68	New Phenoxazine-Based Organic Dyes with Various Acceptors for Dye-Sensitized Solar Cells: Synthesis, Characterization, DSSCs Fabrications and DFT Study. Journal of Computational Biophysics and Chemistry, 2021, 20, 465-476.	1.7	10
69	Concentration-dependent SERS profile of olanzapine on silver and silver-gold metallic substrates. Chemical Papers, 2021, 75, 6059-6072.	2.2	15
70	Molecular docking, DFT analysis, and dynamics simulation of natural bioactive compounds targeting ACE2 and TMPRSS2 dual binding sites of spike protein of SARS CoV-2. Journal of Molecular Liquids, 2021, 342, 116942.	4.9	28
71	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.	4.9	53
72	Modeling the DFT structural and reactivity studies of a pyrimidine -6-carboxylate derivative with reference to its wavefunction-dependent, MD simulations and evaluation for potential antimicrobial activity. Journal of Molecular Structure, 2021, 1237, 130397.	3.6	20

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73	Genomic variation and point mutations analysis of Indian COVID-19 patient samples submitted in GISAID database. Journal of the Indian Chemical Society, 2021, 98, 100156.	2.8	2
74	Reactivity properties and adsorption behavior of a triazole derivative â€“ DFT and MD simulation studies. Journal of Molecular Liquids, 2021, 341, 117439.	4.9	16
75	Surface enhanced Raman scattering investigation of pioglitazone on silver and silver-gold metal substrates â€“ Experimental analysis and theoretical modeling. Journal of Molecular Structure, 2021, 1244, 130992.	3.6	13
76	Structural and reactivity studies of pravadoline â€“An ionic liquid, with reference to its wavefunction-relative properties using DFT and MD simulation. Journal of Molecular Structure, 2021, 1245, 131074.	3.6	19
77	Spectroscopic and computational study of chromone derivatives with antitumor activity: detailed DFT, QTAIM and docking investigations. SN Applied Sciences, 2021, 3, 1.	2.9	5
78	Synthesis, spectral properties, chemical descriptors and light harvesting studies of a new bioactive azo imidazole compound. Journal of Molecular Structure, 2020, 1199, 127035.	3.6	75
79	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.	3.9	69
80	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.	3.6	47
81	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.	3.9	26
82	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. Journal of Molecular Structure, 2020, 1205, 127587.	3.6	53
83	Intricate spectroscopic profiling, light harvesting studies and other quantum mechanical properties of 3-phenyl-5-isooxazolone using experimental and computational strategies. Journal of Molecular Structure, 2020, 1203, 127461.	3.6	35
84	Spectroscopic, quantum mechanical studies, ligand protein interactions and photovoltaic efficiency modeling of some bioactive benzothiazolinone acetamide analogs. Chemical Papers, 2020, 74, 1957-1964.	2.2	39
85	Conformational analysis and quantum descriptors of two new imidazole derivatives by experimental, DFT, AIM, molecular docking studies and adsorption activity on graphene. Heliyon, 2020, 6, e05182.	3.2	16
86	Detailed spectra, electronic properties, qualitative non-covalent interaction analysis, solvatochromism, docking and molecular dynamics simulations in different solvent atmosphere of cenobamate. Structural Chemistry, 2020, 31, 2475-2485.	2.0	45
87	Spectral analysis and DFT investigation of some benzopyran analogues and their self-assemblies with graphene. Journal of Molecular Liquids, 2020, 317, 113924.	4.9	32
88	Structural (SC-XRD), spectroscopic, DFT, MD investigations and molecular docking studies of a hydrazone derivative. Chemical Data Collections, 2020, 30, 100588.	2.3	7
89	Spectral analysis and detailed quantum mechanical investigation of some acetanilide analogues and their self-assemblies with graphene and fullerene. Journal of Molecular Modeling, 2020, 26, 254.	1.8	17
90	DFT and molecular docking studies of self-assembly of sulfone analogues and graphene. Journal of Molecular Modeling, 2020, 26, 273.	1.8	34

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91	Cocrystals of hydrochlorothiazide with picolinamide, tetramethylpyrazine and piperazine: quantum mechanical studies, docking and modelling of the photovoltaic efficiency for DSSC. Journal of Molecular Modeling, 2020, 26, 256.	1.8	9
92	DFT and MD simulations and molecular docking of co-crystals of octafluoro-1,4-diiodobutane with phenazine and acridine. Structural Chemistry, 2020, 31, 2525-2531.	2.0	7
93	Comprehensive quantum mechanical studies on three bioactive anastrozole based triazole analogues and their SERS active graphene complex. Journal of Molecular Structure, 2020, 1217, 128388.	3.6	49
94	Modeling the conformational preference, spectroscopic properties, UV light harvesting efficiency, biological receptor inhibitory ability and other physico-chemical properties of five imidazole derivatives using quantum mechanical and molecular mechanics tools. Journal of Molecular Liquids, 2020, 310, 112871.	4.9	34
95	Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione. Journal of Molecular Structure, 2019, 1175, 269-279.	3.6	16
96	Cocrystals of pyrazinamide with p-toluenesulfonic and ferulic acids: DFT investigations and molecular docking studies. Journal of Molecular Structure, 2019, 1175, 916-926.	3.6	48
97	Quantum mechanical and photovoltaic studies on the cocrystals of hydrochlorothiazide with isonazid and malonamide. Journal of Molecular Structure, 2019, 1197, 719-726.	3.6	48
98	DFT and molecular docking investigations of oxicam derivatives. Heliyon, 2019, 5, e02175.	3.2	47
99	Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide1,1-dimethyl-3-phenylurea. Heliyon, 2019, 5, e01987.	3.2	46
100	Detailed quantum mechanical, molecular docking, QSAR prediction, photovoltaic light harvesting efficiency analysis of benzil and its halogenated analogues. Heliyon, 2019, 5, e02825.	3.2	37
101	Spectroscopic and Theoretical Studies of Potential Anti-Inflammatory Polycyclic Aromatic Fluorophenyl Substituted Acyclic and Heterocyclic Analogues Synthesized from 4,4â€²-Difluorophenylchalcone. Polycyclic Aromatic Compounds, 2019, , 1-13.	2.6	2
102	Structure, Spectral Features, Bioactivity and Light Harvesting Properties of Methyl and Dimethyl Anthracene: Experimental and First Principle Studies. Polycyclic Aromatic Compounds, 2019, , 1-15.	2.6	9
103	Synthesis, characterization and biological investigation of glycine-based sulfonamide derivative and its complex: Vibration assignment, HOMO â€“ LUMO analysis, MEP and molecular docking. Journal of Molecular Structure, 2019, 1181, 244-252.	3.6	63
104	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.	3.6	59
105	Two neoteric pyrazole compounds as potential anti-cancer agents: Synthesis, electronic structure, physico-chemical properties and docking analysis. Journal of Molecular Structure, 2019, 1181, 455-466.	3.6	75
106	Single crystal XRD, DFT investigations and molecular docking study of 2-((1,5-dimethyl-3-oxo-2-phenyl-2,3-dihydro-1H-pyrazol-4-yl)amino)naphthalene-1,4-dione as a potential anti-cancer lead molecule. Computational Biology and Chemistry, 2019, 78, 153-164.	2.3	39
107	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.	3.6	49
108	Understanding reactivity of two newly synthetized imidazole derivatives by spectroscopic characterization and computational study. Journal of Molecular Structure, 2018, 1158, 176-196.	3.6	56

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109	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.	3.6	22
110	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.	3.6	18
111	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.	3.6	11
112	Study on the structure, vibrational analysis and molecular docking of fluorophenyl derivatives using FT-IR and density functional theory computations. Journal of Molecular Structure, 2018, 1164, 172-179.	3.6	16
113	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. Journal of Molecular Structure, 2018, 1155, 184-195.	3.6	16
114	A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene â€“ A frequently used benzene derivative. Journal of Molecular Structure, 2018, 1151, 245-255.	3.6	51
115	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.	3.6	19
116	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.	3.6	42
117	Synthesis, characterization and computational studies of semicarbazide derivative. Journal of Molecular Liquids, 2018, 272, 481-495.	4.9	48
118	Two novel imidazole derivatives â€“ Combined experimental and computational study. Journal of Molecular Structure, 2018, 1173, 221-239.	3.6	10
119	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.	3.6	83
120	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.	3.6	53
121	Molecular structure, spectroscopic, dielectric and thermal study, nonlinear optical properties, natural bond orbital, HOMO-LUMO and molecular docking analysis of (C6Cl2O4) (C10H14N2F)2Â·2H2O. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 204, 328-339.	3.9	37
122	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.	3.6	48
123	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.	3.6	6
124	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. Journal of Molecular Structure, 2017, 1134, 814-827.	3.6	11
125	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. Journal of Molecular Structure, 2017, 1135, 1-14.	3.6	18
126	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. Journal of Molecular Structure, 2017, 1137, 589-605.	3.6	10

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127	Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures. Journal of Molecular Structure, 2017, 1141, 495-511.	3.6	43
128	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.	3.6	13
129	Synthesis, crystal structure analysis, spectral investigations, DFTÂcomputations 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.	3.6	20
130	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.	3.6	42
131	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.	3.6	9
132	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.	3.6	22
133	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.	3.6	18
134	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.	3.6	4
135	Vibrational spectroscopic investigations and molecular docking studies of biologically active 2-[4-(4-phenylbutanamido)phenyl]-5-ethylsulphonyl-benzoxazole. Journal of Molecular Structure, 2017, 1148, 119-133.	3.6	12
136	Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1H-benzoimidazole.3H2O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies. Journal of Molecular Structure, 2017, 1149, 602-612.	3.6	10
137	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.	3.6	11
138	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.	3.6	35
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