Y Sheena Mary

List of Publications by Year in Descending Order

198 papers	3,374 citations	33 h-index	42 g-index
211 ext. papers	4,139 ext. citations	3.3 avg, IF	5.99 L-index

#	Paper	IF	Citations
198	Theoretical and experimental investigation of a pyrazole derivative- solvation effects, reactivity analysis and MD simulations. *Chemical Physics Letters*, **2022**, 793, 139469	2.5	0
197	Evidence of cluster formation of pyrrole with mixed silver metal clusters, Agx-My (x = 4,5, y = 2/1 and M = Au/Ni/Cu) using DFT/SERS analysis. *Computational and Theoretical Chemistry*, **2022**, 1208, 113569	2	7
196	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	4.4	6
195	DFT analysis of valproic acid adsorption onto Al/B-N/P nanocages with solvent effects.. *Journal of Molecular Modeling*, **2022**, 28, 98	2	2
194	A foundational theoreticalAlE(E = N, P) adsorption and quinolone docking study: cage-quinolone pairs, optics and possible therapeutic and diagnostic applications.. *Journal of Biomolecular Structure and Dynamics*, **2022**, 1-17	3.6	2
193	Co-crystals of ethenzamide with 2-nitrobenzoic acid - Conformational analysis, MD simulations and DFT investigations. *Journal of the Indian Chemical Society*, **2022**, 99, 100439		
192	Spectroscopic analyses on an azatricycloderivative by DFT with different solvents, reactivity analysis and MD simulations. *Journal of Molecular Structure*, **2022**, 1260, 132845	3.4	
191	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	6	3
190	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*, **2022**, 1-12	3.6	0
189	Selective detection of F ion and SO2 molecule: An experimental and DFT study. *Journal of Molecular Liquids*, **2022**, 359, 119329	6	0
188	DFT Study of 6-amino-3-(1-hydroxyethyl) pyridine-2,4-diol (AHP) Adsorption on Coronene. *Journal of Molecular Liquids*, **2022**, 119436	6	0
187	Computational Study of Furosemide-Piperazine (FS PZ) and 2,3,5,6-tetramethylpyrazine (FS-TP) Co-Crystals. *Journal of Molecular Liquids*, **2022**, 119537	6	1
186	Adsorption of Diospyrin on the surface of CC/AlN/AlP/GaN Nanotubes: A DFT investigation. *Journal of Molecular Liquids*, **2022**, 360, 119472	6	1
185	Understanding the mechanism of thioguanine's binding to Ag6 and bimetallic (Ag3Au3 and Ag3Cu3) clusters. *Journal of Molecular Structure*, **2022**, 1265, 133415	3.4	1
184	Adsorption of a thione bioactive derivative over different silver/gold clusters - DFT investigations. *Computational and Theoretical Chemistry*, **2021**, 1207, 113497	2	4
183	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*, **2021**, 118061	6	0
182	Adsorption properties of dacarbazine with graphene/fullerene/metal nanocages - Reactivity, spectroscopic and SERS analysis. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2021**, 120677	4.4	2

181	Adsorption behavior and solvent effects of an adamantane-triazole derivative on metal clusters DFT simulation studies. *Journal of Molecular Liquids*, **2021**, 345, 118242	6	7
180	Theoretical model study of adsorbed antimalarial-graphene dimers: doping effects, photophysical parameters, intermolecular interactions, edge adsorption, and SERS. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-12	3.6	4
179	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	3.6	23
178	Optoelectronic properties of the newly designed 1,3,5-triazine derivatives with isatin, chalcone and acridone moieties. *Computational and Theoretical Chemistry*, **2021**, 1197, 113160	2	4
177	Spectroscopic investigations, concentration dependent SERS, and molecular docking studies of a hydroxybenzylidene derivative. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-13	3.6	2
176	Adsorption of adipic acid in Al/B-N/P nanocages: DFT investigations. *Journal of Molecular Modeling*, **2021**, 27, 113	2	14
175	Spectroscopic and DFT investigations of 8-hydroxy quinoline-5-sulfonic acid-5-chloro-8-hydroxyquinoline cocrystal. *Chemical Papers*, **2021**, 75, 3387-3399	1.9	1
174	DFT, docking, MD simulation, and vibrational spectra with SERS analysis of a benzoxazole derivative: an anti-cancerous drug. *Chemical Papers*, **2021**, 75, 4269-4284	1.9	0
173	DFT computational study of trihalogenated aniline derivatives adsorption onto graphene/fullerene/fullerene-like nanocages, XY (X = Al, B, and Y = N, P). *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-14	3.6	7
172	Investigation of reactive properties of an antiviral azatricyclo derivative DFT, MD and docking simulations. *Journal of Molecular Structure*, **2021**, 1230, 129937	3.4	3
171	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	3.4	8
170	Theoretical investigation on the reactive and interaction properties of sorafenib DFT, AIM, spectroscopic and Hirshfeld analysis, docking and dynamics simulation. *Journal of Molecular Liquids*, **2021**, 330, 115652	6	16
169	Modeling the structural and reactivity properties of hydrazono methyl-4H-chromen-4-one derivatives-wavefunction-dependent properties, molecular docking, and dynamics simulation studies. *Journal of Molecular Modeling*, **2021**, 27, 186	2	6
168	Concentration and solvent dependent SERS, DFT, MD simulations and molecular docking studies of a thioxothiazolidine derivative with antimicrobial properties. *Journal of Molecular Liquids*, **2021**, 329, 115582	6	9
167	Investigation of reactive properties, adsorption on fullerene, DFT, molecular dynamics simulation of an anthracene derivative targeting dihydrofolate reductase and human dUTPase. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-10	3.6	2
166	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*, **2021**, 1-13	3.6	0
165	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	2
164	Investigation of the reactivity properties of a thiourea derivative with anticancer activity by DFT and MD simulations. *Journal of Molecular Modeling*, **2021**, 27, 217	2	5

163	Theoretical Studies on the Structure and Various Physico-Chemical and Biological Properties of a Terphenyl Derivative with Immense Anti-Protozoan Activity. *Polycyclic Aromatic Compounds*, **2021**, 41, 825-840	1.3	37
162	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	4.4	14
161	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	4.4	14
160	DFT, SERS-concentration and solvent dependent and docking studies of a bioactive benzenesulfonamide derivative. *Journal of Molecular Structure*, **2021**, 1228, 129680	3.4	9
159	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	1.8	5
158	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	2.1	9
157	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	4.4	7
156	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	4.4	6
155	Biological perspective of a triazine derivative with isatin/chalcone/acridone: DFT and docking investigations. *Structural Chemistry*, **2021**, 32, 19-26	1.8	1
154	Utilization of O/S-doped graphene nanoclusters for ultrasensitive detection of flurane derivatives-DFT investigations. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-8	3.6	1
153	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		0
152	Concentration-dependent SERS profile of olanzapine on silver and silver-gold metallic substrates. *Chemical Papers*, **2021**, 75, 6059-6072	1.9	3
151	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	6	4
150	Stability and reactivity study of bio-molecules brucine and colchicine towards electrophile and nucleophile attacks: Insight from DFT and MD simulations. *Journal of Molecular Liquids*, **2021**, 335, 116192	6	22
149	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	3.4	10
148	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		1
147	Reactivity properties and adsorption behavior of a triazole derivative DFT and MD simulation studies. *Journal of Molecular Liquids*, **2021**, 341, 117439	6	6
146	Surface enhanced Raman scattering investigation of pioglitazone on silver and silver-gold metal substrates Experimental analysis and theoretical modeling. *Journal of Molecular Structure*, **2021**, 1244, 130992	3.4	1

145	Structural and reactivity studies of pravadoline A an ionic liquid, with reference to its wavefunction-relative properties using DFT and MD simulation. *Journal of Molecular Structure*, **2021**, 1245, 131074	3.4	7
144	Spectroscopic and computational study of chromone derivatives with antitumor activity: detailed DFT, QTAIM and docking investigations. *SN Applied Sciences*, **2021**, 3, 1	1.8	2
143	Detailed Quantum Mechanical Studies on Three Bioactive Benzimidazole Derivatives and Their Raman Enhancement on Adsorption over Graphene Sheets. *Polycyclic Aromatic Compounds*, **2020**, 1-10	1.3	11
142	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*, **2020**, 1-11	1.3	11
141	Comprehensive quantum mechanical studies on three bioactive anastrozole based triazole analogues and their SERS active graphene complex. *Journal of Molecular Structure*, **2020**, 1217, 128388	3.4	30
140	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, 113271	6	22
139	Theoretical Studies into the Spectral Characteristics, Biological Activity, and Photovoltaic Cell Efficiency of Four New Polycyclic Aromatic Chalcones. *Polycyclic Aromatic Compounds*, **2020**, 1-15	1.3	2
138	Hybrid and bioactive cocrystals of pyrazinamide with hydroxybenzoic acids: Detailed study of structure, spectroscopic characteristics, other potential applications and noncovalent interactions using SAPT. *Journal of Molecular Structure*, **2020**, 1202, 127316	3.4	32
137	Spectral characterization, thermochemical studies, periodic SAPT calculations and detailed quantum mechanical profiling various physico-chemical properties of 3,4-dichlorodiuron. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 228, 117580	4.4	18
136	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. *Journal of Molecular Structure*, **2020**, 1205, 127587	3.4	29
135	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	3.4	26
134	Spectroscopic, quantum mechanical studies, ligand protein interactions and photovoltaic efficiency modeling of some bioactive benzothiazolinone acetamide analogs. *Chemical Papers*, **2020**, 74, 1957-1964	1.9	25
133	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	3.6	8
132	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	1.8	27
131	Spectral analysis and DFT investigation of some benzopyran analogues and their self-assemblies with graphene. *Journal of Molecular Liquids*, **2020**, 317, 113924	6	16
130	Understanding reactivity of a triazole derivative and its interaction with graphene and doped/undoped-coronene-a DFT study. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-11	3.6	5
129	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*, **2020**, 1-11	1.3	6
128	Structural (SC-XRD), spectroscopic, DFT, MD investigations and molecular docking studies of a hydrazone derivative. *Chemical Data Collections*, **2020**, 30, 100588	2.1	4

127	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	2	11
126	DFT and molecular docking studies of self-assembly of sulfone analogues and graphene. *Journal of Molecular Modeling*, **2020**, 26, 273	2	25
125	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	2	7
124	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	1.8	5
123	Synthesis, spectral properties, chemical descriptors and light harvesting studies of a new bioactive azo imidazole compound. *Journal of Molecular Structure*, **2020**, 1199, 127035	3.4	52
122	Exploring the detailed spectroscopic characteristics, chemical and biological activity of two cyanopyrazine-2-carboxamide derivatives using experimental and theoretical tools. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 224, 117414	4.4	53
121	Synthesis, conformational, characterization and reactivity study of 1,7-bis(4-bromophenyl)heptane-1,7-dione. *Journal of Molecular Structure*, **2019**, 1175, 269-279	3.4	14
120	Cocrystals of pyrazinamide with p-toluenesulfonic and ferulic acids: DFT investigations and molecular docking studies. *Journal of Molecular Structure*, **2019**, 1175, 916-926	3.4	33
119	Quantum mechanical and photovoltaic studies on the cocrystals of hydrochlorothiazide with isonazid and malonamide. *Journal of Molecular Structure*, **2019**, 1197, 719-726	3.4	43
118	DFT and molecular docking investigations of oxicam derivatives. *Heliyon*, **2019**, 5, e02175	3.6	39
117	Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide1,1-dimethyl-3-phenylurea. *Heliyon*, **2019**, 5, e01987	3.6	36
116	Detailed quantum mechanical, molecular docking, QSAR prediction, photovoltaic light harvesting efficiency analysis of benzil and its halogenated analogues. *Heliyon*, **2019**, 5, e02825	3.6	29
115	Quantum Mechanical Studies of Three Aromatic Halogen-Substituted Bioactive Sulfonamidobenzoxazole Compounds with Potential Light Harvesting Properties. *Polycyclic Aromatic Compounds*, **2019**, 1-17	1.3	16
114	Spectroscopic and Theoretical Studies of Potential Anti-Inflammatory Polycyclic Aromatic Fluorophenyl Substituted Acyclic and Heterocyclic Analogues Synthesized from 4,4?-Difluorophenylchalcone. *Polycyclic Aromatic Compounds*, **2019**, 1-13	1.3	2
113	Structure, Spectral Features, Bioactivity and Light Harvesting Properties of Methyl and Dimethyl Anthracene: Experimental and First Principle Studies. *Polycyclic Aromatic Compounds*, **2019**, 1-15	1.3	8
112	Synthesis, characterization and biological investigation of glycine-based sulfonamide derivative and its complex: Vibration assignment, HOMO LUMO analysis, MEP and molecular docking. *Journal of Molecular Structure*, **2019**, 1181, 244-252	3.4	52
111	Synthesis and spectroscopic study of two new pyrazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential. *Journal of Molecular Structure*, **2019**, 1181, 599-612	3.4	44
110	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	3.4	51

109	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	3.6	27
108	Spectroscopic analysis and molecular docking of imidazole derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations. *Journal of Molecular Structure*, **2018**, 1158, 156-175	3.4	41
107	Understanding reactivity of two newly synthetized imidazole derivatives by spectroscopic characterization and computational study. *Journal of Molecular Structure*, **2018**, 1158, 176-196	3.4	49
106	Spectroscopic characterization of hydroxyquinoline derivatives with bromine and iodine atoms and theoretical investigation by DFT calculations, MD simulations and molecular docking studies. *Journal of Molecular Structure*, **2018**, 1167, 95-106	3.4	13
105	Synthesis, spectroscopic analyses, chemical reactivity and molecular docking study and anti-tubercular activity of pyrazine and condensed oxadiazole derivatives. *Journal of Molecular Structure*, **2018**, 1164, 459-469	3.4	14
104	Spectroscopic characterization of 8-hydroxy-5-nitroquinoline and 5-chloro-8-hydroxy quinoline and investigation of its reactive properties by DFT calculations and molecular dynamics simulations. *Journal of Molecular Structure*, **2018**, 1164, 525-538	3.4	11
103	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	3.4	11
102	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. *Journal of Molecular Structure*, **2018**, 1155, 184-195	3.4	16
101	A complete computational and spectroscopic study of 2-bromo-1, 4-dichlorobenzene □A frequently used benzene derivative. *Journal of Molecular Structure*, **2018**, 1151, 245-255	3.4	24
100	Synthesis and spectroscopic study of three new oxadiazole derivatives with detailed computational evaluation of their reactivity and pharmaceutical potential. *Journal of Molecular Structure*, **2018**, 1173, 469-480	3.4	70
99	Molecular dynamic simulations, ALIE surface, Fukui functions geometrical, molecular docking and vibrational spectra studies of tetra chloro p and m-xylene. *Journal of Molecular Structure*, **2018**, 1171, 253-267	3.4	27
98	Molecular structure, spectroscopic, dielectric and thermal study, nonlinear optical properties, natural bond orbital, HOMO-LUMO and molecular docking analysis of (CClO) (CHNF)□2HO. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 204, 328-339	4.4	20
97	Synthesis, spectroscopic analyses (FT-IR and NMR), vibrational study, chemical reactivity and molecular docking study and anti-tubercular activity of condensed oxadiazole and pyrazine derivatives. *Journal of Molecular Structure*, **2018**, 1156, 657-674	3.4	13
96	Spectroscopic analysis of 8-hydroxyquinoline derivatives and investigation of its reactive properties by DFT and molecular dynamics simulations. *Journal of Molecular Structure*, **2018**, 1156, 336-347	3.4	32
95	Synthesis, characterization and computational studies of semicarbazide derivative. *Journal of Molecular Liquids*, **2018**, 272, 481-495	6	27
94	Two novel imidazole derivatives □Combined experimental and computational study. *Journal of Molecular Structure*, **2018**, 1173, 221-239	3.4	10
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. *Journal of Molecular Structure*, **2017**, 1134, 668-680	3.4	25
92	Spectroscopic and reactive properties of a newly synthesized quinazoline derivative: Combined experimental, DFT, molecular dynamics and docking study. *Journal of Molecular Structure*, **2017**, 1134, 863-881	3.4	5

91	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. *Journal of Molecular Structure*, **2017**, 1134, 814-827	3.4	10
90	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. *Journal of Molecular Structure*, **2017**, 1135, 1-14	3.4	13
89	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. *Journal of Molecular Structure*, **2017**, 1137, 589-605	3.4	9
88	Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures. *Journal of Molecular Structure*, **2017**, 1141, 495-511	3.4	36
87	Insight into the reactive properties of newly synthesized 1,2,4-triazole derivative by combined experimental (FT-IR and FR-Raman) and theoretical (DFT and MD) study. *Journal of Molecular Structure*, **2017**, 1141, 542-550	3.4	11
86	Synthesis, crystal structure analysis, spectral investigations, DFT computations and molecular dynamics and docking study of 4-benzyl-5-oxomorpholine-3-carbamide, a potential bioactive agent. *Journal of Molecular Structure*, **2017**, 1134, 25-39	3.4	12
85	Spectroscopic, DFT, molecular dynamics and molecular docking study of 1-butyl-2-(4-hydroxyphenyl)-4,5-dimethyl-imidazole 3-oxide. *Journal of Molecular Structure*, **2017**, 1134, 330-344	3.4	29
84	Synthesis, vibrational spectroscopic investigations, molecular docking, antibacterial studies and molecular dynamics study of 5-[(4-nitrophenyl)acetamido]-2-(4-tert-butylphenyl)benzoxazole. *Journal of Molecular Structure*, **2017**, 1133, 557-573	3.4	7
83	Spectroscopic analysis of 8-hydroxyquinoline-5-sulphonic acid and investigation of its reactive properties by DFT and molecular dynamics simulations. *Journal of Molecular Structure*, **2017**, 1150, 540-552	3.4	20
82	Synthesis, XRD single crystal structure analysis, vibrational spectral analysis, molecular dynamics and molecular docking studies of 2-(3-methoxy-4-hydroxyphenyl) benzothiazole. *Journal of Molecular Structure*, **2017**, 1148, 282-292	3.4	16
81	Investigation of reactive and spectroscopic properties of oxobutanoic acid derivative: Combined spectroscopic, DFT, MD and docking study. *Journal of Molecular Structure*, **2017**, 1148, 266-275	3.4	4
80	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	3.4	9
79	Supramolecular architecture of 5-bromo-7-methoxy-1-methyl-1 H -benzoimidazole.3H 2 O: Synthesis, spectroscopic investigations, DFT computation, MD simulations and docking studies. *Journal of Molecular Structure*, **2017**, 1149, 602-612	3.4	7
78	Conformational, vibrational and DFT studies of a newly synthesized arylpiperazine-based drug and evaluation of its reactivity towards the human GABA receptor. *Journal of Molecular Structure*, **2017**, 1147, 266-280	3.4	7
77	Vibrational spectroscopic analysis of cyanopyrazine-2-carboxamide derivatives and investigation of their reactive properties by DFT calculations and molecular dynamics simulations. *Journal of Molecular Structure*, **2017**, 1131, 1-15	3.4	29
76	Molecular conformational analysis, reactivity, vibrational spectral analysis and molecular dynamics and docking studies of 6-chloro-5-isopropylpyrimidine-2,4(1H,3H)-dione, a potential precursor to bioactive agent. *Journal of Molecular Structure*, **2017**, 1127, 427-436	3.4	8
75	FT-IR, FT-Raman and NMR characterization of 2-isopropyl-5-methylcyclohexyl quinoline-2-carboxylate and investigation of its reactive and optoelectronic properties by molecular dynamics simulations and DFT calculations. *Journal of Molecular Structure*, **2017**, 1127, 124-137	3.4	38
74	Spectroscopic characterization of 4-[2-(5-Ethylpyridin-2-yl)ethoxy]benzaldehyde oxime and investigation of its reactive properties by DFT calculations and molecular dynamics simulations. *Journal of Molecular Structure*, **2017**, 1128, 245-256	3.4	22

73	Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxymethyl benzimidazole. *Journal of Molecular Structure*, **2017**, 1129, 86-97	3.4	12
72	Spectroscopic characterization of 1-[3-(1 H -imidazol-1-yl)propyl]-3-phenylthiourea and assessment of reactive and optoelectronic properties employing DFT calculations and molecular dynamics simulations. *Journal of Molecular Structure*, **2017**, 1129, 72-85	3.4	35
71	Reactive, spectroscopic and antimicrobial assessments of 5-[(4-methylphenyl) acetamido]-2-(4-tert-butylphenyl)benzoxazole: Combined experimental and computational study. *Journal of Molecular Structure*, **2017**, 1128, 694-706	3.4	12
70	Vibrational spectroscopic studies, Fukui functions, HOMO-LUMO, NLO, NBO analysis and molecular docking study of (E)-1-(1,3-benzodioxol-5-yl)-4,4-dimethylpent-1-en-3-one, a potential precursor to bioactive agents. *Journal of Molecular Structure*, **2016**, 1123, 375-383	3.4	38
69	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	3.7	38
68	FT-IR, FT-Raman and molecular docking study of ethyl 4-(2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)acetamido)benzoate. *Journal of Molecular Structure*, **2016**, 1111, 9-18	3.4	15
67	DFT and experimental (FT-IR and FT-Raman) investigation of vibrational spectroscopy and molecular docking studies of 2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)-N-(3,4,5-trimethoxyphenyl) acetamide. *Journal of Molecular Structure*, **2016**, 1113, 133-145	3.4	40
66	Spectroscopic analysis (FT-IR, FT-Raman and NMR) and molecular docking study of ethyl 2-(4-oxo-3-phenethyl-3,4-dihydroquinazolin-2-ylthio)-acetate. *Journal of Molecular Structure*, **2016**, 1119, 451-461	3.4	12
65	Spectral investigations, DFT computations and molecular docking studies of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-{3-[4-(2-methylphenyl)piperazin-1-yl]propyl}-4-azatricyclo[5.2.1.02,6]dec-8-ene-3,5 *Journal of Molecular Structure*, **2015**, 1098, 130-145	3.4	12
64	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO–LUMO analysis and molecular docking study of 1-hydroxy-4,5,8-tris(4-methoxyphenyl) anthraquinone. *Journal of Physics and Chemistry of Solids*, **2015**, 87, 110-121	3.9	14
63	Molecular conformational analysis, vibrational spectra, NBO, NLO analysis and molecular docking study of bis[(E)-anthranyl-9-acrylic]anhydride based on density functional theory calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 151, 350-9	4.4	11
62	Vibrational spectra, HOMO, LUMO, NBO, MEP analysis and molecular docking study of 2,2-diphenyl-4-(piperidin-1-yl)butanamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 150, 543-56	4.4	48
61	Spectroscopic investigations, NBO, HOMO–LUMO, NLO analysis and molecular docking of 5-(adamantan-1-yl)-3-anilinomethyl-2,3-dihydro-1,3,4-oxadiazole-2-thione, a potential bioactive agent. *Journal of Molecular Structure*, **2015**, 1096, 1-14	3.4	36
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50	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO, NBO, MEP analysis and molecular docking study of 2-[(4-chlorobenzyl)sulfanyl]-4-(2-methylpropyl)-6-(phenylsulfanyl)-pyrimidine-5-carbonitrile, a	4.4	15
49	Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-[3-(4-phenylpiperazin-1-yl)propyl]-4-azatricyclo[5.2.1.0(2,6)]dec-8-ene-3,5-dione by density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 124, 500-13	4.4	12
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