Y Sheena Mary

List of Publications by Citations

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	FT-IR, FT-raman and SERS spectra of L-proline. *Journal of the Iranian Chemical Society*, **2009**, 6, 138-144	2	73
197	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
196	FT-IR, FT-Raman, SERS and computational study of 5-ethylsulphonyl-2-(o-chlorobenzyl)benzoxazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 617-25	4.4	64
195	Molecular structure, FT-IR, vibrational assignments, HOMO-LUMO analysis and molecular docking study of 1-[5-(4-Bromophenyl)-3-(4-fluorophenyl)-4,5-dihydro-1H-pyrazol-1-yl]ethanone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt B, 473-82	4.4	61
194	Vibrational spectroscopic studies and ab initio calculations of 5-nitro-2-(p-fluorophenyl)benzoxazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 71, 566-71	4.4	53
193	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
192	FT-IR, NBO, HOMO-LUMO, MEP analysis and molecular docking study of 1-[3-(4-Fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazol-1-yl]ethanone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt B, 483-93	4.4	52
191	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
190	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
189	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
188	Vibrational spectroscopic, molecular structure, first hyperpolarizability and NBO studies of 4Smethylbiphenyl-2-carbonitrile. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 98, 91-9	4.4	50
187	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
186	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
185	IR, Raman, SERS and computational study of 2-(benzylsulfanyl)-3,5-dinitrobenzoic acid. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 113, 28-36	4.4	45
184	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
183	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
182	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

181	Vibrational spectroscopic studies and computational study of quinoline-2-carbaldehyde benzoyl hydrazone. *Journal of Molecular Structure*, **2010**, 973, 36-46	3.4	41
180	Molecular structure, FT-IR, NBO, HOMO and LUMO, MEP and first order hyperpolarizability of (2E)-1-(2,4-Dichlorophenyl)-3-(3,4,5-trimethoxyphenyl)prop-2-en-1-one by HF and density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 81-92	4.4	40
179	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
178	DFT and molecular docking investigations of oxicam derivatives. *Heliyon*, **2019**, 5, e02175	3.6	39
177	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
176	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
175	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
174	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
173	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
172	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
171	Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide1,1-dimethyl-3-phenylurea. *Heliyon*, **2019**, 5, e01987	3.6	36
170	Vibrational spectroscopic studies and computational study of 4-fluoro-N-(2?-hydroxy-4?-nitrophenyl)phenylacetamide. *Journal of Molecular Structure*, **2011**, 994, 223-231	3.4	36
169	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
168	Molecular conformational analysis, vibrational spectra, NBO, NLO, HOMO-LUMO and molecular docking studies of ethyl 3-(E)-(anthracen-9-yl)prop-2-enoate based on density functional theory calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 150, 533-42	4.4	35
167	Theoretical investigations on the molecular structure, vibrational spectral, HOMO-LUMO and NBO analysis of 9-[3-(Dimethylamino)propyl]-2-trifluoro-methyl-9H-thioxanthen-9-ol. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 132, 491-501	4.4	34
166	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
165	FT-IR, molecular structure, first order hyperpolarizability, HOMO and LUMO analysis, MEP and NBO analysis of 2-(4-chlorophenyl)-2-oxoethyl 3-nitrobenzoate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 126, 208-19	4.4	33
164	Vibrational spectroscopic and quantum chemical calculations of (E)-N-Carbamimidoyl-4-((naphthalen-1-yl-methylene)amino)benzene sulfonamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 87, 29-39	4.4	32

163	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
162	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
161	Infrared spectrum, structural and optical properties and molecular docking study of 3-(4-fluorophenyl)-5-phenyl-4,5-dihydro-1H-pyrazole-1-carbaldehyde. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 138, 529-38	4.4	31
160	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMO-LUMO analysis and molecular docking study of 2-(Adamantan-1-yl)-5-(4-nitrophenyl)-1,3,4-oxadiazole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 973-83	4.4	31
159	FT-IR, FT-Raman, surface enhanced Raman scattering and computational study of 2-(p-fluorobenzyl)-6-nitrobenzoxazole. *Journal of Molecular Structure*, **2012**, 1012, 22-30	3.4	31
158	Spectroscopic investigations and computational study of 2-[acetyl(4-bromophenyl)carbamoyl]-4-chlorophenyl acetate. *Journal of Raman Spectroscopy*, **2010**, 41, 707-716	2.3	31
157	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
156	FT-IR, FT-Raman and computational study of (E)-N-carbamimidoyl-4-((4-methoxybenzylidene)amino)benzenesulfonamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 92, 84-90	4.4	30
155	Vibrational spectra and computational study of 3-amino-2-phenyl quinazolin-4(3H)-one. *Journal of Molecular Structure*, **2010**, 963, 137-144	3.4	30
154	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
153	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
152	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
151	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
150	Infrared and Raman spectroscopic analyses and theoretical computation of 4-butyl-1-(4-hydroxyphenyl)-2-phenyl-3,5-pyrazolidinedione. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 94, 101-9	4.4	28
149	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
148	FT-IR, FT-Raman and computational study of 1H-2,2-dimethyl-3H-phenothiazin-4[10H]-one. *Journal of Molecular Structure*, **2011**, 985, 316-322	3.4	27
147	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
146	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

145	Synthesis, characterization and computational studies of semicarbazide derivative. *Journal of Molecular Liquids*, **2018**, 272, 481-495	6	27
144	Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-(3-chlorophenyl)prop-2-enoic anhydride based on density functional theory calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 131, 471-83	4.4	26
143	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
142	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
141	FT-IR, FT-Raman, and computational calculations of 4-chloro-2-(3-chlorophenyl carbamoyl)phenyl acetate. *Journal of Raman Spectroscopy*, **2009**, 40, 2176-2186	2.3	25
140	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
139	DFT and molecular docking studies of self-assembly of sulfone analogues and graphene. *Journal of Molecular Modeling*, **2020**, 26, 273	2	25
138	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
137	Concentration and pH dependent SERS spectra of sulfanilic acid sodium salt on colloidal silver particles. *Journal of Raman Spectroscopy*, **2010**, 41, 944-951	2.3	24
136	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
135	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	6	22
134	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
133	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
132	Theoretical investigations on the molecular structure, vibrational spectra, HOMO-LUMO analyses and NBO study of 1-[(Cyclopropylmethoxy)methyl]-5-ethyl-6-(4-methylbenzyl)-1,2,3,4-tetrahydropyrimidine-2,4-dione. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 122, 438-50	4.4	21
131	Molecular conformational analysis, vibrational spectra, NBO analysis and first hyperpolarizability of (2E)-3-phenylprop-2-enoic anhydride based on density functional theory calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128, 638-46	4.4	21
130	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
129	Spectroscopic (FT-IR, FT-Raman) investigations and quantum chemical calculations of 1,7,8,9-tetrachloro-10,10-dimethoxy-4-{3-[4-(3-methoxyphenyl)piperazin-1-yl]propyl}-4-azatricyclo[5.2.1.0(2,6)]dec-8-ene-3,5-dione. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 129, 438-50	4.4	20
128	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

127	Spectroscopic investigation (FT-IR, FT-Raman and SERS), vibrational assignments, HOMO-LUMO analysis and molecular docking study of Opipramol. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 137, 547-59	4.4	19
126	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
125	FT-IR, molecular structure, HOMO-LUMO, MEP, NBO analysis and first order hyperpolarizability of Methyl 4,4?-difluoro-5Smethoxy-1,1S3S1?-terphenyl-4Scarboxylate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 133, 480-8	4.4	17
124	Combined spectroscopic, DFT, TD-DFT and MD study of newly synthesized thiourea derivative. *Journal of Molecular Structure*, **2018**, 1155, 184-195	3.4	16
123	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
122	Spectral analysis and DFT investigation of some benzopyran analogues and their self-assemblies with graphene. *Journal of Molecular Liquids*, **2020**, 317, 113924	6	16
121	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
120	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
119	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
118	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 potential chemotherapeutic agent. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 138, 73-84	4.4	15
117	FT-IR, FT-Raman spectroscopy and computational study of N-carbamimidoyl-4-{[(E)-((2-hydroxyphenyl)methylidene]amino}benzenesulfonamide. *Journal of Molecular Structure*, **2011**, 992, 77-83	3.4	15
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115	Molecular structure, FT-IR, vibrational assignments, HOMO-LUMO, MEP, NBO analysis and molecular docking study of ethyl-6-(4-chlorophenyl)-4-(4-fluorophenyl)-2-oxocyclohex-3-ene-1-carboxylate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 138, 73-84	4.4	14
114	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
113	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
112	Vibrational Spectroscopic Investigations of 4-nitropyrocatechol. *Oriental Journal of Chemistry*, **2012**, 28, 937-941	0.8	14
111	Adsorption of adipic acid in Al/B-N/P nanocages: DFT investigations. *Journal of Molecular Modeling*, **2021**, 27, 113	2	14
110	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

109	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
108	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. *Journal of Molecular Structure*, **2017**, 1135, 1-14	3.4	13
107	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
106	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
105	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
104	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
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102	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*	4.4	12
101	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
100	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
99	Quantum chemical DFT study of 4-azatricyclo [5.2.2.0(2,6)] undecane-3,5,8-trione. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2010**, 75, 1559-65	4.4	12
98	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
97	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
96	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
95	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
94	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
93	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
92	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

91	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
90	Newly synthesized dihydroquinazoline derivative from the aspect of combined spectroscopic and computational study. *Journal of Molecular Structure*, **2017**, 1134, 814-827	3.4	10
89	Molecular structure, FT-IR, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2-(4-chlorophenyl)-2-oxoethyl 3-methylbenzoate by HF and density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128, 327-36	4.4	10
88	Acid-base properties, FT-IR, FT-Raman spectroscopy and computational study of 1-(pyrid-4-yl)piperazine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014** , 121, 436-44	4.4	10
87	Two novel imidazole derivatives Combined experimental and computational study. *Journal of Molecular Structure*, **2018**, 1173, 221-239	3.4	10
86	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
85	Towards the new heterocycle based molecule: Synthesis, characterization and reactivity study. *Journal of Molecular Structure*, **2017**, 1137, 589-605	3.4	9
84	Vibrational spectroscopic studies and molecular docking of 10,10-Dimethylanthrone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 135, 652-61	4.4	9
83	Vibrational spectra, molecular structure, NBO, HOMO-LUMO and first order hyperpoalarizability analysis of 1,4-bis(4-formylphenyl)anthraquinone by density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 131, 225-34	4.4	9
82	Vibrational spectroscopic and computational study of 1,7,8,9-Tetrachloro-4-(4-bromo-butyl)-10,10-dimethoxy-4-aza-tricyclo[5.2.1.0(2,6)] dec-8-ene-3,5-dione. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**,	4.4	9
81	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
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