Y Sheena Mary

List of Publications by Year
in descending order

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204 papers	5,003 citations	100601 38 h-index	223390 49 g-index
211 all docs	211 docs citations	211 times ranked	2077 citing authors

#	Article	IF	Citations
1	FT-IR, FT-raman and SERS spectra of L-proline. Journal of the Iranian Chemical Society, 2009, 6, 138-144.	1.2	90
2	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.	1.8	83
3	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, 617-625.	2.0	77
4	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.	1.8	75
5	Synthesis, spectral properties, chemical descriptors and light harvesting studies of a new bioactive azo imidazole compound. Journal of Molecular Structure, 2020, 1199, 127035.	1.8	75
6	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.	2.0	69
7	Molecular structure, FT-IR, vibrational assignments, HOMOâ€“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, 473-482.	2.0	67
8	FT-IR, NBO, HOMOâ€“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, 483-493.	2.0	65
9	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.	1.8	63
10	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, 543-556.	2.0	59
11	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.	1.8	59
12	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.	1.8	58
13	Vibrational spectroscopic studies and ab initio calculations of 5-nitro-2-(p-fluorophenyl)benzoxazole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 566-571.	2.0	57
14	Vibrational spectroscopic, molecular structure, first hyperpolarizability and NBO studies of 4â€²-methylbiphenyl-2-carbonitrile. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 98, 91-99.	2.0	56
15	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.	2.0	56
16	Understanding reactivity of two newly synthetized imidazole derivatives by spectroscopic characterization and computational study. Journal of Molecular Structure, 2018, 1158, 176-196.	1.8	56
17	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.	2.0	53
18	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.	1.8	53

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19	Experimental and computational analysis of 1-(4-chloro-3-nitrophenyl)-3-(3,4-dichlorophenyl)thiourea. Journal of Molecular Structure, 2020, 1205, 127587.	1.8	53
20	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.	2.3	53
21	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.	1.8	51
22	Spectroscopic investigations, NBO, HOMOâ€“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.	1.8	50
23	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.	1.8	49
24	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.	1.8	49
25	Comprehensive quantum mechanical studies on three bioactive anastrozole based triazole analogues and their SERS active graphene complex. Journal of Molecular Structure, 2020, 1217, 128388.	1.8	49
26	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.	1.8	48
27	Synthesis, characterization and computational studies of semicarbazide derivative. Journal of Molecular Liquids, 2018, 272, 481-495.	2.3	48
28	Cocrystals of pyrazinamide with p-toluenesulfonic and ferulic acids: DFT investigations and molecular docking studies. Journal of Molecular Structure, 2019, 1175, 916-926.	1.8	48
29	Quantum mechanical and photovoltaic studies on the cocrystals of hydrochlorothiazide with isonazid and malonamide. Journal of Molecular Structure, 2019, 1197, 719-726.	1.8	48
30	DFT and molecular docking investigations of oxicam derivatives. Heliyon, 2019, 5, e02175.	1.4	47
31	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.	1.8	47
32	Vibrational spectroscopic studies and computational study of quinoline-2-carbaldehyde benzoyl hydrazone. Journal of Molecular Structure, 2010, 973, 36-46.	1.8	46
33	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
34	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
35	Conformational profile, vibrational assignments, NLO properties and molecular docking of biologically active herbicide1,1-dimethyl-3-phenylurea. Heliyon, 2019, 5, e01987.	1.4	46
36	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.	1.0	45

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37	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.	1.4	44
38	Modification of benzoxazole derivative by bromine-spectroscopic, antibacterial and reactivity study using experimental and theoretical procedures. Journal of Molecular Structure, 2017, 1141, 495-511.	1.8	43
39	Theoretical investigations on the molecular structure, vibrational spectral, HOMOâ€“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.	2.0	42
40	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.	1.8	42
41	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.	1.8	42
42	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.	2.3	40
43	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.	2.0	39
44	Molecular conformational analysis, vibrational spectra, NBO, NLO, HOMOâ€“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, 533-542.	2.0	39
45	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
46	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.	1.1	39
47	Spectroscopic, quantum mechanical studies, ligand protein interactions and photovoltaic efficiency modeling of some bioactive benzothiazolinone acetamide analogs. Chemical Papers, 2020, 74, 1957-1964.	1.0	39
48	Vibrational spectroscopic studies and computational study of 4-fluoro-N-(2â€²-hydroxy-4â€²-nitrophenyl)phenylacetamide. Journal of Molecular Structure, 2011, 994, 223-231.	1.8	38
49	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.	2.0	37
50	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.	1.8	37
51	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“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, 973-983.	2.0	37
52	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.	2.0	37
53	Detailed quantum mechanical, molecular docking, QSAR prediction, photovoltaic light harvesting efficiency analysis of benzil and its halogenated analogues. Heliyon, 2019, 5, e02825.	1.4	37
54	Spectroscopic investigations and computational study of 2â€[acetyl(4â€bromophenyl)carbamoyl]â€4â€chlorophenyl acetate. Journal of Raman Spectroscopy, 2010, 41, 707-716.	1.2	36

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55	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, 208-219.	2.0	36
56	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, 529-538.	2.0	36
57	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.	2.0	36
58	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
59	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.	1.8	35
60	Adsorption of adipic acid in Al/B-N/P nanocages: DFT investigations. Journal of Molecular Modeling, 2021, 27, 113.	0.8	35
61	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.	2.3	35
62	DFT and molecular docking studies of self-assembly of sulfone analogues and graphene. Journal of Molecular Modeling, 2020, 26, 273.	0.8	34
63	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.	2.3	34
64	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.	2.3	34
65	Concentration and pH dependent SERS spectra of sulfanilic acid sodium salt on colloidal silver particles. Journal of Raman Spectroscopy, 2010, 41, 944-951.	1.2	33
66	Vibrational spectra and computational study of 3-amino-2-phenyl quinazolin-4(3H)-one. Journal of Molecular Structure, 2010, 963, 137-144.	1.8	32
67	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, 471-483.	2.0	32
68	Spectroscopic investigation (FT-IR, FT-Raman and SERS), vibrational assignments, HOMOâ€“LUMO analysis and molecular docking study of Opipramol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 137, 547-559.	2.0	32
69	Spectral analysis and DFT investigation of some benzopyran analogues and their self-assemblies with graphene. Journal of Molecular Liquids, 2020, 317, 113924.	2.3	32
70	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.	2.0	30
71	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, 101-109.	2.0	29
72	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.	1.8	28

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73	Quantum Mechanical Studies of Three Aromatic Halogen-Substituted Bioactive Sulfonamidobenzoxazole Compounds with Potential Light Harvesting Properties. Polycyclic Aromatic Compounds, 2021, 41, 1563-1579.	1.4	28
74	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.	2.0	28
75	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.	2.3	28
76	Evidence of cluster formation of pyrrole with mixed silver metal clusters, Agx-My (xÂ=Â4,5, yÂ=Â2/1 and) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	28
77	FTâ€IR, FTâ€Raman, and computational calculations of 4â€chloroâ€2â€(3â€chlorophenyl carbamoyl)phenyl acetate. Journal of Raman Spectroscopy, 2009, 40, 2176-2186.	1.2	27
78	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, 638-646.	2.0	27
79	Theoretical investigations on the molecular structure, vibrational spectra, HOMOâ€“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, 133, 639-650.	2.0	26
80	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
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.	2.0	26
82	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.	2.0	24
83	Adsorption of Diospyrin on the surface of CC/AlN/AlP/GaN Nanotubes: A DFT investigation. Journal of Molecular Liquids, 2022, 360, 119472.	2.3	24
84	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[5.2.1.02,6]dec-8-ene-3,5-dione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 129, 438-450.	2.0	23
85	DFT, SERS-concentration and solvent dependent and docking studies of a bioactive benzenesulfonamide derivative. Journal of Molecular Structure, 2021, 1228, 129680.	1.8	23
86	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.	1.8	22
87	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.	1.8	22
88	FT-IR, molecular structure, HOMOâ€“LUMO, MEP, NBO analysis and first order hyperpolarizability of Methyl 4,4â€³-difluoro-5â€²-methoxy-1,1â€²:3â€²,1â€³-terphenyl-4â€²-carboxylate. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 480-488.	2.0	21
89	Investigation of the reactivity properties of a thiourea derivative with anticancer activity by DFT and MD simulations. Journal of Molecular Modeling, 2021, 27, 217.	0.8	21
90	Adsorption behavior and solvent effects of an adamantane-triazole derivative on metal clusters â€“ DFT simulation studies. Journal of Molecular Liquids, 2022, 345, 118242.	2.3	21

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91	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[5.2.1.02,6]dec-8-ene-3,5-dione by density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 124, 500-513.	2.0	20
92	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“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.	1.9	20
93	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.	1.8	20
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, 2022, 42, 1260-1270.	1.4	20
95	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.	2.0	20
96	Optoelectronic properties of the newly designed 1,3,5-triazine derivatives with isatin, chalcone and acridone moieties. Computational and Theoretical Chemistry, 2021, 1197, 113160.	1.1	20
97	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.	2.0	20
98	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.	1.8	20
99	DFT study of 6-amino-3-(1-hydroxyethyl) pyridine-2,4-diol (AHP) adsorption on Coronene. Journal of Molecular Liquids, 2022, 360, 119436.	2.3	20
100	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.	1.8	19
101	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.	1.4	19
102	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.	2.0	19
103	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.	1.8	19
104	New quinolone derivative: Spectroscopic characterization and reactivity study by DFT and MD approaches. Journal of Molecular Structure, 2017, 1135, 1-14.	1.8	18
105	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.	1.8	18
106	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.	1.8	18
107	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.	2.0	18
108	Adsorption of a thione bioactive derivative over different silver/gold clusters â€“ DFT investigations. Computational and Theoretical Chemistry, 2022, 1207, 113497.	1.1	18

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109	Spectroscopic investigation (FT-IR and FT-Raman), vibrational assignments, HOMOâ€“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, 139, 413-424.	2.0	17
110	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.	1.8	17
111	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.	0.8	17
112	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.	3.2	17
113	Vibrational Spectroscopic Investigations of 4-nitropyrocatechol. Oriental Journal of Chemistry, 2012, 28, 937-941.	0.1	17
114	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.	2.0	17
115	FT-IR, FT-Raman spectroscopy and computational study of		

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127	1-Alkyl-1-methylpiperazine-1,4-diium salts: Synthetic, acidâ€“base, XRD-analytical, FT-IR, FT-Raman spectral and quantum chemical study. Journal of Molecular Structure, 2015, 1094, 210-236.	1.8	15
128	Molecular structure, FT-IR, vibrational assignments, HOMOâ€“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.	2.0	15
129	Vibrational spectroscopic analysis, molecular dynamics simulations and molecular docking study of 5-nitro-2-phenoxymethyl benzimidazole. Journal of Molecular Structure, 2017, 1129, 86-97.	1.8	15
130	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.	1.8	15
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132	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, 350-359.	2.0	14
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