S Muthu

List of Publications by Year in Descending Order

221 papers	3,172 citations	33 h-index	44 g-index
232 ext. papers	4,252 ext. citations	3.3 avg, IF	6.17 L-index

#	Paper	IF	Citations
221	Molecular structure spectroscopic Elucidation, IEFPCM solvation (UV–Vis, MEP, FMO, NBO, NLO), molecular docking and biological assessment studies of lepidine (4-Methylquinoline). *Journal of Molecular Liquids*, **2022**, 345, 118249	6	5
220	Theoretical electron excitation study in liquid phase (protic, aprotic, non-polar) and inter and intra molecular reactivity of 2-hydroxy-5-[1-hydroxy-2-(4-phenylbutan-2-ylamino) ethyl] benzamide. *Journal of the Indian Chemical Society*, **2022**, 99, 100372		1
219	Quantum computational, spectroscopic investigations on N-(2-((2-chloro-4,5-dicyanophenyl)amino)ethyl)-4-methylbenzenesulfonamide by DFT/TD-DFT with different solvents, molecular docking and drug-likeness researches. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **2022**, 639, 128311	5.1	35
218	Exploration of experimental, theoretical, Hirshfeld surface, molecular docking and electronic excitation studies of Menadione: A potent anti-cancer agent. *Journal of Molecular Liquids*, **2022**, 351, 118670	6	1
217	Spectroscopic, quantum mechanical investigation and molecular docking study of 2-amino-5-chloro-3-nitropyridine. *Materials Today: Proceedings*, **2022**, 50, 2711-2719	1.4	0
216	Vibrational (FT-IR, FT Raman), electronic and docking studies and wave function analysis with quantum chemical computation on 3-Bromophenyl acetic acid: A potential amidase inhibitor. *Materials Today: Proceedings*, **2022**, 50, 2853-2864	1.4	
215	Spectroscopic, quantum mechanical, electronic excitation properties (Ethanol solvent), DFT investigations and molecular docking analysis of an anti-cancer drug Bendamustine. *Journal of Molecular Structure*, **2022**, 1253, 132211	3.4	3
214	Structural examination, theoretical calculations, and pharmaceutical scanning of a new tetralone based chalcone derivative. *Journal of Molecular Structure*, **2022**, 1253, 132296	3.4	1
213	Synthesis and investigation of anti-COVID19 ability of ferrocene Schiff base derivatives by quantum chemical and molecular docking.. *Journal of Molecular Structure*, **2022**, 1253, 132242	3.4	1
212	Anti-microbial activity, molecular profiling, electronic properties and molecular docking investigations of 5[1-hydroxy2[(isopropylamino)ethyl] benzene1,3diol. *Journal of Molecular Structure*, **2022**, 1247, 131299	3.4	5
211	Computational, spectroscopic and molecular docking investigation on a bioactive anti-cancer drug: 2-Methyl-8-nitro quinoline. *Journal of Molecular Structure*, **2022**, 1247, 131414	3.4	1
210	Computational Investigation on Structural and Reactive Sites (HOMO-LUMO, MEP, NBO, NPA, ELF, LOL, RDG) Identification, Pharmacokinetic (ADME) Properties and Molecular Docking Investigation of (E)-4-((4-chlorobenzylidene) amino) Benzene Sulfonamide Compound. *Analytical Chemistry Letters*, **2022**, 12, 58-76	1	3
209	Evaluation of Vibrational, Electronic, Topology, Reactivity, Bioactivity, Bioavailability and Blood-Brain Barrier Score of 1-(2,6-dimethylphenoxy)propan-2-amine-A DFT, Spectro-scopic and Molecular Docking Approach. *Analytical Chemistry Letters*, **2022**, 12, 102-118	1	
208	Molecular Structure, Spectroscopic Assessment, PDOS, Topology Evaluation and Docking Studies of 2-Chloro-5-nitrobenzophenone. *Analytical Chemistry Letters*, **2022**, 12, 198-220	1	
207	Investigations on Spectroscopic, ADMET Properties and drug-likeness, Molecular docking, Chemical properties of (2E)-3-(biphenyl-4-yl)-1-(2,4-dichlorophenyl)-prop-2-en-1-one by combined Density-functional theory. *Journal of Molecular Structure*, **2022**, 132973	3.4	1
206	Synthesis, spectral property, IEF-PCM solvation, anti-microbial evaluation and molecular docking studies of 6 amino-2-(4 nitrophenyl)-1H-benzimidazole. *Journal of Molecular Liquids*, **2022**, 352, 118756	6	1
205	Structural, electronic properties (different solvents), chemical reactivity, ELF, LOL, spectroscopic insights, molecular docking and in vitro anticancer activity studies on methyl (4-nitro-1-imidazolyl)acetate. *Journal of the Indian Chemical Society*, **2022**, 99, 100438		0

204	Experimental spectra, electronic energies (liquid and gaseous phases) quantum computational strategies and potential biological activity studies of (1E, 4E)-1, 5-bis (4-methoxyphenyl) penta-1,4-dien-3-one: An antiviral agent. *Journal of Molecular Liquids*, **2022**, 356, 119012	6	0
203	Theoretical spectroscopic electronic elucidation with different solvents (IEFPCM model), biological assessment and molecular docking studies on Moroxydine-Antiviral drug agent. *Journal of Molecular Liquids*, **2022**, 355, 118946	6	1
202	Conformational stability, quantum computational, spectroscopic, molecular docking and molecular dynamic simulation study of 2-hydroxy-1-naphthaldehyde. *Journal of Molecular Structure*, **2022**, 1259, 132755	3.4	2
201	Synthesis, Spectroscopic, Molecular Docking and inhibitory activity of 6-Bromo-2-(4-chlorophenyl)-1H-benzimidazole- a DFT approach. *Journal of Molecular Structure*, **2022**, 1261, 132815	3.4	1
200	Experimental spectroscopic, Molecular structure, Electronic solvation, Biological prediction and Topological analysis of 2, 4, 6-tri (propan-2-yl) benzenesulfonyl chloride: an antidepressant agent. *Journal of Molecular Liquids*, **2022**, 119166	6	1
199	Donor acceptor groups effect, polar protic solvents influence on electronic properties and reactivity of 2-Chloropyridine-4-carboxylic acid. *Journal of the Indian Chemical Society*, **2022**, 99, 100478		0
198	Computational investigation into structural, topological, electronic properties, and biological evaluation of spiro[1H-indole-3,2?-3H-1,3-benzothiazole]-2-one. *Journal of Molecular Liquids*, **2022**, 359, 119234	6	1
197	Structural, spectral inspection, electronic properties in different solvents, Fukui functions, 6-acetyl-2H-1,4-benzoxazin-3(4H)-one Multiple sclerosis and auto immune disorders therapeutics. *Journal of Molecular Liquids*, **2022**, 359, 119248	6	1
196	Density functional studies and spectroscopic analysis (FT-IR, FT-Raman, UV isible, and NMR) with molecular docking approach on an anticancer and antifungal drug 4-hydroxy-3-methoxybenzaldehyde. *Journal of Molecular Structure*, **2022**, 1264, 133134	3.4	
195	Molecular docking evaluation and spectroscopic study of 2-amino-1,4-benzenedisulfonic acid using the IEFPCM model, electronic properties of different solvents. *Journal of the Indian Chemical Society*, **2022**, 100543		
194	Quantum computational, spectroscopic (FT-IR, NMR and UV Vis) profiling, Hirshfeld surface, Molecular docking and dynamics simulation studies on Pyridine-2,6-dicarbonyl dichloride. *Journal of Molecular Structure*, **2022**, 133374	3.4	3
193	Electronic properties (in different solvents), spectroscopic progression and evaluation on 4-morpholinepropane sulfonic acid along with molecular docking analysis. *Journal of Molecular Liquids*, **2021**, 349, 118107	6	1
192	Theoretical conformations studies on 2-Acetyl-gamma-butyrolactone structure and stability in aqueous phase and the solvation effects on electronic properties by quantum computational methods. *Computational and Theoretical Chemistry*, **2021**, 113534	2	2
191	Structural, vibrational, electronic properties, hirshfeld surface analysis topological and molecular docking studies of N-[2-(diethylamino)ethyl]-2-methoxy-5-methylsulfonylbenzamide. *Heliyon*, **2021**, 7, e08186	3.6	5
190	Electronic properties of solvents (Water, Benzene, Ethanol) using IEFPCM model, spectroscopic exploration with drug likeness and assessment of molecular docking on 1-Octanesulfonic Acid Sodium Salt. *Journal of Molecular Liquids*, **2021**, 344, 117719	6	1
189	Structure, hirshfeld surface studies, optical and mechanical analysis on a third-order nonlinear optical crystal 2-amino-6-methylpyridin-1-ium 2-chloro-4-nitrobenzoate (2A6M2C4N). *Optical Materials*, **2021**, 122, 111731	3.3	0
188	Spectroscopic, quantum computational, molecular docking and biological parameters of 4-phenylbutyrophenone: a neuroleptic agent. *Chemical Papers*, **2021**, 75, 3931-3948	1.9	
187	Exploring the molecular structure, vibrational spectroscopic, quantum chemical calculation and molecular docking studies of curcumin: A potential PI3K/AKT uptake inhibitor. *Heliyon*, **2021**, 7, e06646	3.6	2

186	Computational evaluation on molecular structure (Monomer, Dimer), RDG, ELF, electronic (HOMO-LUMO, MEP) properties, and spectroscopic profiling of 8-Quinolinesulfonamide with molecular docking studies. *Computational and Theoretical Chemistry*, **2021**, 1198, 113169	2	17
185	Speculative assessment, molecular composition, PDOS, topology exploration (ELF, LOL, RDG), ligand-protein interactions, on 5-bromo-3-nitropyridine-2-carbonitrile. *Heliyon*, **2021**, 7, e07061	3.6	4
184	Vibrational spectra and Wavefunction investigation for antidepressant drug of Amoxapine based on quantum computational studies. *Chemical Data Collections*, **2021**, 33, 100699	2.1	9
183	Experimental and theoretical spectroscopic (FT-IR, FT-Raman, UV-VIS) analysis, natural bonding orbitals and molecular docking studies on 2-bromo-6-methoxynaphthalene: A potential anti-cancer drug. *Heliyon*, **2021**, 7, e07213	3.6	3
182	Spectroscopic (FT-IR, FT-Raman, UV-Vis) molecular structure, electronic, molecular docking, and thermodynamic investigations of indole-3-carboxylic acid by DFT method. *Journal of Molecular Structure*, **2021**, 1234, 130182	3.4	8
181	Vibrational spectroscopy, quantum computational and molecular docking studies on 2-chloroquinoline-3-carboxaldehyde. *Heliyon*, **2021**, 7, e07529	3.6	4
180	Elaborated molecular structure, molecular docking and vibrational spectroscopic investigation of N-((4-aminophenyl)sulfonyl)benzamide with Density functional theory. *Chemical Data Collections*, **2021**, 31, 100609	2.1	6
179	Molecular structure, spectroscopic (FT-IR, FT-Raman, NMR), HOMO-LUMO, chemical reactivity, AIM, ELF, LOL and Molecular docking studies on 1-Benzyl-4-(N-Boc-amino)piperidine. *Journal of Molecular Structure*, **2021**, 1230, 129657	3.4	18
178	Computational spectroscopic investigations on structural validation with IR and Raman experimental evidence, projection of ultraviolet-visible excitations, natural bond orbital interpretations, and molecular docking studies under the biological investigation on N-Benzyloxycarbonyl-L-Aspartic acid 1-Benzyl ester. *Chemical Data Collections*, **2021**, 31, 100622	2.1	11
177	Molecular docking, spectroscopic, and quantum chemical studies on aromatic heterocycle tetrakis(4-pyridyl)cyclobutane regioisomers: potential membrane-permeable inhibitors. *Journal of Molecular Modeling*, **2021**, 27, 94	2	2
176	Growth, spectral, optical, electrical and computational analysis of sodium oxalate single crystals. *Heliyon*, **2021**, 7, e06527	3.6	0
175	Theoretical description of green solvents effect on electronic property and reactivity of Tert-butyl 4-formylpiperidine-1-carboxylate. *Computational and Theoretical Chemistry*, **2021**, 1201, 113255	2	3
174	Structural (monomer and dimer), wavefunctional, NCI analysis in aqueous phase, electronic and excited state properties in different solvent atmosphere of 3-{(E)-[(3,4-dichlorophenyl)imino]methyl} benzene-1,2-diol. *Journal of Molecular Liquids*, **2021**, 336, 116335	6	11
173	Phenolic and flavonoid contents in Malva sylvestris and exploration of active drugs as antioxidant and anti-COVID19 by quantum chemical and molecular docking studies. *Journal of Saudi Chemical Society*, **2021**, 25, 101277	4.3	8
172	Computational investigation, comparative approaches, molecular structural, vibrational spectral, non-covalent interaction (NCI), and electron excitations analysis of benzodiazepine derivatives. *Journal of Molecular Modeling*, **2021**, 27, 266	2	5
171	Molecular structure determination, Bioactivity score, Spectroscopic and Quantum computational studies on (E)-N'-(4-Chlorobenzylidene)-2-(napthalen-2-yloxy) acetohydrazide. *Journal of Molecular Structure*, **2021**, 1241, 130558	3.4	8
170	Theoretical investigation on influence of protic and aprotic solvents effect and structural (Monomer, Dimer), Van-der Waals and Hirshfeld surface analysis for clonidine molecule. *Computational and Theoretical Chemistry*, **2021**, 1204, 113397	2	4
169	Facile synthesis of aminoalkyl naphthols and single crystal X-ray, computational studies on 1-[morpholino(thiophen-2-yl)methyl]naphthalen-2-ol. *Journal of Molecular Structure*, **2021**, 1242, 130861	3.4	2

168	Evaluation of electronic and biological interactions between N-[4-(Ethylsulfamoyl)phenyl]acetamide and some polar liquids (IEFPCM solvation model) with Fukui function and molecular docking analysis. *Journal of Molecular Liquids*, **2021**, 340, 117271	6	11
167	Conformational study, FT-IR, FT-Raman, solvent effect on UV□Vis, charge transfer and protein□ligand interactions of Methyl-2-pyrazinecarboxylate. *Journal of Molecular Liquids*, **2021**, 341, 116934	6	5
166	Evaluation of electronic properties in different solvents, spectroscopic exposition (FT-IR, FT-Raman), and molecular docking studies of 5-Chloro-2-hydroxypyridine - insulysin inhibitor. *Journal of Molecular Liquids*, **2021**, 341, 117304	6	1
165	Computational prediction of polar and non-polar solvent effect on the electronic property of N-BOC- Piperidine-4-Carboxylic acid. *Journal of Molecular Liquids*, **2021**, 341, 117222	6	2
164	Probing solvent effect and strong and weak interactions in 2-Nitrophenyl-hydrazine using independent gradient model and Hirshfeld from wave function calculation. *Journal of Molecular Liquids*, **2021**, 341, 117345	6	1
163	Quantum computational studies on optimization, donor-acceptor analysis and solvent effect on reactive sites, global descriptors, non-linear optical parameters of Methyl N-Boc-piperidine-3-carboxylate. *Journal of Molecular Liquids*, **2021**, 343, 117608	6	2
162	Molecular Docking, Structural Examination, Reactive Sites Identification (Homo□lumo, Mep) of 6-Phenylpteridine 2, 4, 7-triamine: Potential Bacterial Inhibitor. *Analytical Chemistry Letters*, **2021**, 11, 886-898	1	1
161	Spectroscopic (FT-IR, FT-Raman, UV-Visible), Quantum Mechanical Based Computational Studies and Molecular Docking Analysis of 2-Amino-3,5-dichloropyridine. *Analytical Chemistry Letters*, **2021**, 11, 848-861	1	
160	Spectroscopic (FT-IR, FT Raman and UV-Vis), Quantum Computational and Molecular Docking studies on Propylthiouracil. *Analytical Chemistry Letters*, **2021**, 11, 771-791	1	0
159	Spectroscopic profiling, DFT computations, molecular docking and molecular dynamic simulation of biologically active 5-isoquinolinesulfonic acid. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-14	3.6	0
158	Spectroscopic (FT-IR, FT-Raman and UV-Vis), computational (ELF, LOL, NBO, HOMO-LUMO, Fukui, MEP) studies and molecular docking on benzodiazepine derivatives- heterocyclic organic arenes. *Chemical Data Collections*, **2020**, 30, 100574	2.1	7
157	Quantum mechanical, spectroscopic and docking studies of (2E)-1-(4-aminophenyl)-3-(4-benzyloxyphenyl)-prop-2-en-1-one Chalcone derivative by density functional theory - A prospective respiratory drug. *Materials Today: Proceedings*, **2020**, 50, 2816-2816	1.4	1
156	Spectroscopic investigations, quantum chemical calculations and molecular docking studies of Mangiferin - an anti-viral agent of H1N1 Influenza virus. *Chemical Data Collections*, **2020**, 30, 100580	2.1	6
155	Quantum chemical calculations, spectroscopic investigation and molecular docking analysis of 4-chloro-N-methylpyridine-2-carboxamide. *Journal of Molecular Structure*, **2020**, 1210, 128053	3.4	3
154	Quantum mechanical computation, spectroscopic exploration and molecular docking analysis of 2-Bromo-4-fluoroacetanilide. *Journal of Molecular Structure*, **2020**, 1220, 128639	3.4	7
153	Molecular structure, spectroscopic (FT-IR, FT-Raman, NMR, UV-VIS), chemical reactivity and biological examinations of Ketorolac. *Journal of Molecular Structure*, **2020**, 1210, 128040	3.4	8
152	Evaluation of vibrational, electronic, reactivity and bioactivity of propafenone□A spectroscopic, DFT and molecular docking approach. *Chemical Data Collections*, **2020**, 26, 100360	2.1	10
151	Spectroscopic elucidation (FT-IR, FT-Raman and UV-visible) with NBO, NLO, ELF, LOL, drug likeness and molecular docking analysis on 1-(2-ethylsulfonylethyl)-2-methyl-5-nitro-imidazole: An antiprotozoal agent. *Computational Biology and Chemistry*, **2020**, 88, 107330	3.6	17

150	Wavefunction analysis, charge transfer and molecular docking studies on famciclovir and entecavir: Potential anti-viral drugs. *Chemical Data Collections*, **2020**, 26, 100353	2.1	2
149	Molecular docking, quantum chemical computational and vibrational studies on bicyclic heterocycle "6-nitro-2,3-dihydro-1,4-benzodioxine": Anti-cancer agent. *Computational Biology and Chemistry*, **2020**, 86, 107226	3.6	6
148	Theoretical and experimental spectroscopic studies of monomeric and dimeric structures of 4-hydroxybenzamide. *Journal of Molecular Structure*, **2020**, 1206, 127742	3.4	1
147	Quantum computational, spectroscopic and molecular docking studies on 2-acetylthiophene and its bromination derivative. *Journal of Molecular Structure*, **2020**, 1212, 128129	3.4	15
146	Spectroscopic (FT-IR, FT-RAMAN, NMR, UV□Vis) investigations, computational analysis and molecular docking study of 5-bromo-2-hydroxy pyrimidine. *Journal of Molecular Structure*, **2020**, 1218, 128494	3.4	14
145	Density functional studies and spectroscopic analysis (FT-IR, FT-Raman, UV□isible, and NMR)with molecular docking approach on an antifibrotic drug Pirfenidone. *Journal of Molecular Structure*, **2020**, 1203, 127394	3.4	8
144	Molecular structure conformational analyses, solvent-electronic studies through theoretical studies and biological profiling of (2E)-1-(3-bromo-2-thienyl)-3-(4-chlorophenyl)-prop-2-en-1-one. *Journal of Molecular Structure*, **2020**, 1202, 127349	3.4	6
143	Co-crystals of urea and hexanedioic acid with third-order nonlinear properties: An experimental and theoretical enquiry. *Journal of Molecular Structure*, **2020**, 1202, 127237	3.4	17
142	Vibrational spectroscopy, reactive site analysis and molecular docking studies on 2-[(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)methoxy]-3-hydroxypropyl (2S)-2-amino-3-methylbutanoate. *Journal of Molecular Structure*, **2020**, 1202, 127274	3.4	9
141	Computational assessment on wave function (ELF, LOL) analysis, molecular confirmation and molecular docking explores on 2-(5-Amino-2- Methylanilino)-4-(3-pyridyl) pyrimidine. *Chemical Data Collections*, **2020**, 29, 100525	2.1	8
140	Investigations on 2-(4-Cyanophenylamino) acetic acid by FT-IR,FT-Raman, NMR and UV-Vis spectroscopy, DFT (NBO, HOMO-LUMO, MEP and Fukui function) and molecular docking studies. *Heliyon*, **2020**, 6, e04976	3.6	21
139	Spectroscopic (FT-IR, FT-Raman) investigations, chemical properties, antimicrobial and molecular docking analyses of 2-hydroxybenzhydrazied. *Materials Today: Proceedings*, **2020**, 50, 2640-2640	1.4	1
138	Spectroscopic (FT-IR and FT-Raman), quantum computational (DFT) and molecular docking studies on 2(E)-(4-N,N-dimethylaminobenzylidene)-5-methylcyclohexanone. *Materials Today: Proceedings*, **2020**, 50, 2695-2695	1.4	2
137	Investigation of spectroscopic (FT-IR, FT-Raman), reactive charge transfer and docking properties of (1S) -(+)-10-Camphorsulfonic acid by density functional method. *Materials Today: Proceedings*, **2020**, 50, 2768-2768	1.4	1
136	PES, molecular structure, spectroscopic (FT-IR, FT-Raman), electronic (UV-Vis, HOMO-LUMO), quantum chemical and biological (docking) studies on a potent membrane permeable inhibitor: dibenzoxepine derivative. *Heliyon*, **2020**, 6, e04724	3.6	14
135	Vibrational spectroscopic, DFT studies and molecular docking on (2R)-2-acetamido-N-benzyl-3-methoxy propanamide as an antineuropathic pain drug. *Materials Today: Proceedings*, **2020**,	1.4	2
134	Quantum mechanical, spectroscopic vibrational analysis, NBO, HOMO-LUMO, and molecular docking studies on 2-Chloroquinoline-3-Carboxamide. *Materials Today: Proceedings*, **2020**, 50, 2655-2655	1.4	1
133	Synthesis, spectroscopic elucidation (FT-IR, FT-Raman, UV□is), electronic properties and biological activities (antimicrobial, docking) of semicarbazide derivative. *Materials Today: Proceedings*, **2020**, 50, 2847-2847	1.4	3

132	Structure-Activity relationship of Quercetin and its Tumor Necrosis Factor Alpha inhibition activity by computational and machine learning methods. *Materials Today: Proceedings*, **2020**,	1.4	2
131	Quantum Chemical, Vibrational Spectroscopic and Molecular Docking Studies of 1-(Diphenylmethyl)Piperazine. *Polycyclic Aromatic Compounds*, **2020**, 1-21	1.3	1
130	Growth, molecular structure and characterization of L-Isoleucinium hydrogen maleate hemihydrate (LIM) NLO single crystal by density function theory. *Materials Today: Proceedings*, **2020**, 50, 2599-2599	1.4	
129	Spectroscopic, quantum chemical calculations, and molecular docking analysis of 3-Chlorophenyl boronic acid. *Spectroscopy Letters*, **2020**, 53, 778-792	1.1	2
128	Spectroscopic theoretical studies and wave function analysis on 1-Phenyl sulfonyl Pyrrole with quantum chemical computation techniques. *Materials Today: Proceedings*, **2020**, 50, 2826-2826	1.4	0
127	Spectroscopic and DFT studies, structural determination, chemical properties and molecular docking of 1-(3-bromo-2-thienyl)-3-[4-(dimethylamino)-phenyl]prop-2-en-1-one. *Journal of Molecular Structure*, **2020**, 1200, 127123	3.4	13
126	Molecular structure interpretation, spectroscopic (FT-IR, FT-Raman), electronic solvation (UV-Vis, HOMO-LUMO and NLO) properties and biological evaluation of (2E)-3-(biphenyl-4-yl)-1-(4-bromophenyl)prop-2-en-1-one: Experimental and computational modeling approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**,	4.4	26
125	Spectroscopic and quantum computational study on naproxen sodium. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 226, 117614	4.4	22
124	Experimental and Quantum Chemical Computational Analysis of Novel N4,N4?-Dimethyl-[1,1?-Biphenyl]-3,3?,4,4?-Tetraamine. *Polycyclic Aromatic Compounds*, **2020**, 1-17	1.3	7
123	A computational and spectroscopic interpretation (FT-IR, FT-Raman, UV□is and NMR) with molecular docking studies on 3-carboxy-2-hydroxy-N, N, N-trimethyl-1-propanaminium hydroxide: A pharmaceutical drug. *Chemical Data Collections*, **2019**, 20, 100191	2.1	8
122	An antipsychotic drug: Spectroscopic identification, structural features, DFT computations and molecular docking studies on 4-(methylamino)-3-nitrobenzoic acid. *Journal of Molecular Structure*, **2019**, 1196, 33-41	3.4	2
121	Spectroscopic, chemical reactivity, molecular docking investigation and QSAR analyses of (2E)-1-(3-bromo-2-thienyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 222, 117190	4.4	10
120	Spectroscopic, quantum computational and molecular docking studies on 1-phenylcyclopentane carboxylic acid. *Computational Biology and Chemistry*, **2019**, 82, 44-56	3.6	21
119	Molecular docking, spectroscopic studies on 4-[2-(Dipropylamino) ethyl]-1,3-dihydro-2H-indol-2-one and QSAR study of a group of dopamine agonists by density functional method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 222, 117185	4.4	5
118	Computational evaluation of the reactivity and pharmaceutical potential of an organic amine: A DFT, molecular dynamics simulations and molecular docking approach. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 222, 117188	4.4	31
117	Spectral, DFT and molecular docking investigations on Etodolac. *Journal of Molecular Structure*, **2019**, 1195, 747-761	3.4	21
116	Spectroscopic and quantum/classical mechanics based computational studies to compare the ability of Andrographolide and its derivative to inhibit Nitric Oxide Synthase. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2019**, 218, 374-387	4.4	21
115	DFT, molecular docking and experimental FT-IR, FT-Raman, NMR inquisitions on □4-chloro-N-(4,5-dihydro-1H-imidazol-2-yl)-6-methoxy-2-methylpyrimidin-5-amine□ Alpha-2-imidazoline receptor agonist antihypertensive agent. *Journal of Molecular Structure*, **2019**, 1186, 468-481	3.4	48

114	Influence of acetyl, hydroxy and methyl functional groups on 2-phenylbutanoic acid by quantum computational, spectroscopic and ligand-protein docking studies. *Journal of Molecular Structure*, **2019**, 1188, 99-109	3.4	18
113	Optical, vibrational (FT-IR and FT-Raman), electronic and molecular docking investigations of 1 Phenyl Isatin. *Optik*, **2019**, 182, 1211-1227	2.5	11
112	Spectroscopic (FT-IR, FT-Raman), quantum mechanical and docking studies on methyl[(3S)-3-(naphthalen-1-yloxy)-3-(thiophen-2-yl)propyl]amine. *Journal of Molecular Structure*, **2019**, 1175, 163-174	3.4	32
111	Vibrational and computational analysis for molecular structure properties of N-(2-(trifluoromethyl)phenyl)acetamide: Density functional theory approach. *Spectroscopy Letters*, **2019**, 52, 563-576	1.1	6
110	Quantum computational, spectroscopic investigations on 6-aminobenzimidazole by DFT/TD-DFT with different solvents and molecular docking studies. *Journal of Molecular Liquids*, **2019**, 296, 111787	6	15
109	Molecular structure, spectroscopic (FT-IR, FT-Raman) studies, Homo□lumo and Fukui function calculations of 2-Acetyl amino-5-bromo- 4 methyl pyridine by density functional theory. *Chemical Data Collections*, **2019**, 24, 100291	2.1	12
108	Spectroscopic, Hirshfeld surface, charge transfer excitation, condensed Fukui function and molecular docking investigations of 1-(3-Bromo-2-thienyl)-3-(4-butoxyphenyl)-prop-2-en-1-one. *Chemical Data Collections*, **2019**, 24, 100309	2.1	2
107	Structure□Activity relationship studies of two dietary flavonoids and their Nitric Oxide Synthase inhibition activity by spectroscopic and quantum/classical computational techniques. *Journal of Theoretical and Computational Chemistry*, **2019**, 18, 1950031	1.8	3
106	Spectroscopic (FT-IR, FT-Raman, NMR) investigation on 2-[(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)methoxy]ethyl(2S)-2-amino-3-methylbutanoate by Density Functional Theory. *Materials Today: Proceedings*, **2019**, 18, 1770-1782	1.4	4
105	Synthesis, characterization, spectroscopic studies, DFT and molecular docking analysis of N, N?-dibutyl-3, 3?-diaminobenzidine. *Journal of Molecular Structure*, **2019**, 1179, 325-335	3.4	9
104	Molecular docking studies, charge transfer excitation and wave function analyses (ESP, ELF, LOL) on valacyclovir : A potential antiviral drug. *Computational Biology and Chemistry*, **2019**, 78, 9-17	3.6	75
103	Quantum mechanical, spectroscopic and molecular docking studies of N-[4-cyano-3-(trifluoromethyl) phenyl]-3-[(4-fluorophenyl)sulfonyl]-2-hydroxy-2-methylpropanamide. *Chemical Data Collections*, **2019**, 19, 100183	2.1	5
102	Laser damage threshold, hardness and third order non-linear optical analysis of potassium dihydrogen phosphate with sodium chloride. *Chemical Data Collections*, **2019**, 19, 100169	2.1	1
101	Structure, spectroscopic study and DFT calculations of 2,6 bis (tri fluro methyl) benzoic acid. *Journal of Molecular Structure*, **2019**, 1177, 401-417	3.4	9
100	Growth and characterization of l -Serine: A promising acentric organic crystal. *Physica B: Condensed Matter*, **2018**, 541, 32-42	2.8	11
99	Quantum computational studies, spectroscopic (FT-IR, FT-Raman and UV□Vis) profiling, natural hybrid orbital and molecular docking analysis on 2,4 Dibromoaniline. *Journal of Molecular Structure*, **2018**, 1160, 393-405	3.4	68
98	Vibrational spectroscopic (FT-IR, FT-Raman) and quantum mechanical study of 4-(2-chlorophenyl)-2-ethyl-9-methyl-6H-thieno[3,2-f] [1,2,4]triazolo[4,3-a][1,4] diazepine. *Journal of Molecular Structure*, **2018**, 1157, 519-529	3.4	56
97	Spectroscopic investigation, hirshfeld surface analysis and molecular docking studies on anti-viral drug entecavir. *Journal of Molecular Structure*, **2018**, 1164, 447-458	3.4	43

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