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List of Publications by Citations

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	Synthesis, spectroscopic (FT-IR, FT-Raman, NMR, UV–Visible), NLO, NBO, HOMO-LUMO, Fukui function and molecular docking study of (E)-1-(5-bromo-2-hydroxybenzylidene)semicarbazide. *Journal of Molecular Structure*, **2017**, 1141, 284-298	3.4	92
220	Quantum mechanical study and spectroscopic (FT-IR, FT-Raman, 13C, 1H, UV) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 4-[(4-aminobenzene) sulfonyl] aniline by ab initio HF and density functional method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 93, 154-63	4.4	88
219	Molecular orbital studies (hardness, chemical potential and electrophilicity), vibrational investigation and theoretical NBO analysis of 4-4'-(1H-1,2,4-triazol-1-yl methylene) dibenzonitrile based on abinitio and DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 120, 237-51	4.4	80
218	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
217	Quantum mechanical, spectroscopic and docking studies of 2-Amino-3-bromo-5-nitropyridine by Density Functional Method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2017**, 181, 153-163	4.4	74
216	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
215	Synthesis, structural, spectroscopic studies, NBO analysis, NLO and HOMO-LUMO of 4-methyl-N-(3-nitrophenyl)benzene sulfonamide with experimental and theoretical approaches. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 159-70	4.4	65
214	Vibrational spectra and normal coordinate analysis of 2-hydroxy-3-(2-methoxyphenoxy) propyl carbamate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 132, 313-25	4.4	58
213	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
212	Electronic absorption, vibrational spectra, non-linear optical properties, NBO analysis and thermodynamic properties of 9-[(2-hydroxyethoxy) methyl] guanine molecule by density functional method. *Solid State Sciences*, **2013**, 16, 90-101	3.4	51
211	Molecular structure analysis and spectroscopic characterization of 9-methoxy-2H-furo[3,2-g]chromen-2-one with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 137, 721-9	4.4	50
210	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
209	Molecular structure, vibrational spectra, AIM, HOMO-LUMO, NBO, UV, first order hyperpolarizability, analysis of 3-thiophenecarboxylic acid monomer and dimer by Hartree-Fock and density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt C, 1227-42	4.4	48
208	Vibrational spectroscopic investigation on the structure of 2-ethylpyridine-4-carbothioamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 93, 214-22	4.4	47
207	Synthesis, spectroscopic (FT-IR, FT-Raman, NMR, UV–Visible), first order hyperpolarizability, NBO and molecular docking study of (E)-1-(4-bromobenzylidene)semicarbazide. *Journal of Molecular Structure*, **2017**, 1128, 481-492	3.4	47
206	Quantum mechanical and spectroscopic (FT-IR, FT-Raman,1H,13C NMR, UV-Vis) studies, NBO, NLO, HOMO, LUMO and Fukui function analysis of 5-Methoxy-1H-benzo[d]imidazole-2(3H)-thione by DFT studies. *Journal of Molecular Structure*, **2017**, 1130, 511-521	3.4	46
205	Vibrational assignments and electronic structure calculations for 6-thioguanine. *Journal of Raman Spectroscopy*, **2009**, 40, 1675-1681	2.3	45

204	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
203	Molecular docking, vibrational spectroscopy studies of (RS)-2-(tert-butylamino)-1-(3-chlorophenyl)propan-1-one: A potential adrenaline uptake inhibitor. *Journal of Molecular Structure*, **2018**, 1173, 251-260	3.4	43
202	Quantum mechanical, spectroscopic study (FT-IR and FT - Raman), NBO analysis, HOMO-LUMO, first order hyperpolarizability and docking studies of a non-steroidal anti-inflammatory compound. *Journal of Molecular Structure*, **2018**, 1156, 645-656	3.4	42
201	Quantum mechanical and spectroscopic (FT-IR, FT-Raman) study, NBO analysis, HOMO-LUMO, first order hyperpolarizability and molecular docking study of methyl[(3R)-3-(2-methylphenoxy)-3-phenylpropyl]amine by density functional method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 189, 289-303	4.4	41
200	Synthesis, X-ray structural, characterization, NBO and HOMO-LUMO analysis using DFT study of 4-methyl-N-(naphthalene-1-yl)benzene sulfonamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 96, 657-67	4.4	41
199	Quantum mechanical study and spectroscopic (FT-IR, FT-Raman, (13)C, (1)H) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2-acetoxybenzoic acid by density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 136 Pt C, 1260-8	4.4	39
198	Molecular structure, vibrational spectra, first order hyper polarizability, NBO and HOMO–LUMO analysis of 4-amino-3(4-chlorophenyl) butanoic acid. *Solid State Sciences*, **2012**, 14, 476-487	3.4	39
197	Spectroscopic studies (FTIR, FT-Raman and UV), potential energy surface scan, normal coordinate analysis and NBO analysis of (2R,3R,4R,5S)-1-(2-hydroxyethyl)-2-(hydroxymethyl) piperidine-3,4,5-triol by DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 30-40	4.4	38
196	Electronic absorption, vibrational spectra, nonlinear optical properties, NBO analysis and thermodynamic properties of N-(4-nitro-2-phenoxyphenyl) methanesulfonamide molecule by ab initio HF and density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 186-96	4.4	37
195	FTIR and Raman spectra, electronic spectra and normal coordinate analysis of N,N-dimethyl-3-phenyl-3-pyridin-2-yl-propan-1-amine by DFT method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 127, 439-53	4.4	36
194	Molecular structure, normal coordinate analysis, harmonic vibrational frequencies, NBO, HOMO-LUMO analysis and detonation properties of (S)-2-(2-oxopyrrolidin-1-yl) butanamide by density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 118, 702-15	4.4	36
193	Quantum mechanical, spectroscopic studies (FT-IR, FT-Raman, NMR, UV) and normal coordinates analysis on 3-([2-(diaminomethyleneamino) thiazol-4-yl] methylthio)-N'-sulfamoylpropanimidamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 108, 307-18	4.4	36
192	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**, 638, 128311	5.1	35
191	Spectroscopic investigation (FTIR spectrum), NBO, HOMO-LUMO energies, NLO and thermodynamic properties of 8-Methyl-N-vanillyl-6-nonenamideby DFT methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 146, 177-86	4.4	34
190	Spectroscopic and molecular structure (monomeric and dimeric structure) investigation of 2-[(2-hydroxyphenyl) carbonyloxy] benzoic acid by DFT method: A combined experimental and theoretical study. *Journal of Molecular Structure*, **2013**, 1038, 145-162	3.4	34
189	Synthesis, structure, spectroscopic studies (FT-IR, FT-Raman and UV), normal coordinate, NBO and NLO analysis of salicylaldehyde p-chlorophenylthiosemicarbazone. *Journal of Molecular Structure*, **2015**, 1081, 400-412	3.4	33
188	Vibrational spectroscopy investigation using ab initio and density functional theory on p-anisaldehyde. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2008**, 70, 550-6	4.4	33
187	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

186	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
185	Vibrational spectroscopy investigation using ab initio and density functional theory on flucytosine. *Journal of Raman Spectroscopy*, **2007**, 38, 1523-1531	2.3	30
184	Spectroscopic (FT-IR, FT-Raman) investigation, topology (ESP, ELF, LOL) analyses, charge transfer excitation and molecular docking (dengue, HCV) studies on ribavirin. *Chemical Data Collections*, **2018**, 17-18, 236-250	2.1	28
183	Spectroscopic (FT-IR, FT Raman) and quantum mechanical study on N-(2,6-dimethylphenyl)-2-{4-[2-hydroxy-3-(2-methoxyphenoxy)propyl]piperazin-1-yl}acetamide. *Journal of Molecular Structure*, **2018**, 1171, 268-278	3.4	28
182	Vibrational spectra, molecular structure, natural bond orbital, first order hyperpolarizability, thermodynamic analysis and normal coordinate analysis of Salicylaldehyde p-methylphenylthiosemicarbazone by density functional method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 134, 453-64	4.4	27
181	Vibrational spectroscopic study and NBO analysis on tranexamic acid using DFT method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 129, 184-92	4.4	27
180	Growth and characterization of dl-Mandelic acid (C6H5CH(OH)CO2H) single crystal for third-order nonlinear optical applications. *Journal of Molecular Structure*, **2017**, 1148, 314-321	3.4	26
179	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	4.4	26
178	Investigation on 1-Acetyl-4-(4-hydroxyphenyl) piperazine an anti-fungal drug by spectroscopic, quantum chemical computations and molecular docking studies. *Journal of Molecular Structure*, **2018**, 1173, 583-595	3.4	23
177	Spectroscopic studies (FTIR, FT-Raman and UV-Visible), normal coordinate analysis, NBO analysis, first order hyper polarizability, HOMO and LUMO analysis of (1R)-N-(Prop-2-yn-1-yl)-2,3-dihydro-1H-inden-1-amine molecule by ab initio HF and density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**,	4.4	23
176	Spectroscopic and quantum computational study on naproxen sodium. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2020**, 226, 117614	4.4	22
175	Spectroscopic, quantum computational and molecular docking studies on 1-phenylcyclopentane carboxylic acid. *Computational Biology and Chemistry*, **2019**, 82, 44-56	3.6	21
174	Spectral, DFT and molecular docking investigations on Etodolac. *Journal of Molecular Structure*, **2019**, 1195, 747-761	3.4	21
173	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
172	Quantum mechanical, spectroscopic studies and molecular docking analysis on 5,5-diphenylimidazolidine-2,4-dione. *Journal of Molecular Structure*, **2017**, 1149, 487-498	3.4	21
171	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
170	Molecular structural, non-linear optical, second order perturbation and Fukui studies of Indole-3-Aldehyde using density functional calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 106, 299-309	4.4	20
169	Molecular structure and spectroscopic characterization of ethyl 4-aminobenzoate with experimental techniques and DFT quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 112, 169-81	4.4	20

168	Vibrational spectroscopic studies, normal co-ordinate analysis, first order hyperpolarizability, HOMO-LUMO of midodrine by using density functional methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 134, 127-42	4.4	19
167	Spectroscopic profiling (FT-IR, FT-Raman, NMR and UV-Vis), autoxidation mechanism (H-BDE) and molecular docking investigation of 3-(4-chlorophenyl)-N,N-dimethyl-3-pyridin-2-ylpropan-1-amine by DFT/TD-DFT and molecular dynamics: A potential SSRI drug. *Computational Biology and Chemistry*, **2018**, 77, 131-145	3.6	19
166	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
165	Growth, spectroscopic studies, and third order non-linear optical analysis of an organic dicarboxylic acid based single crystal: Urea Oxalic acid. *Chinese Journal of Physics*, **2018**, 56, 1449-1466	3.5	18
164	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
163	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
162	Vibrational and electronic absorption spectroscopic profiling, natural hybrid orbital, charge transfer, electron localization function and molecular docking analysis on 3-amino-3-(2-nitrophenyl) propionic acid. *Journal of Molecular Structure*, **2018**, 1171, 733-746	3.4	17
161	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
160	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
159	FT-IR, FT-Raman spectra and ab initio HF and DFT calculations of 7-chloro-5-(2-chlorophenyl)-3-hydroxy-2,3-dihydro-1H-1,4-benzodiazepin-2-one. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 120, 185-94	4.4	16
158	Synthesis, spectroscopic (FT-IR, FT-Raman, NMR, UV–Visible), Fukui function, antimicrobial and molecular docking study of (E)-1-(3-bromobenzylidene)semicarbazide by DFT method. *Journal of Molecular Structure*, **2017**, 1130, 374-384	3.4	16
157	Molecular structure, vibrational spectra, first order hyper polarizability, NBO and HOMO-LUMO analysis of 2-amino-5-bromo-benzoic acid methyl ester. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 137, 1374-86	4.4	16
156	Quantum computational, spectroscopic and molecular docking studies on 2-acetylthiophene and its bromination derivative. *Journal of Molecular Structure*, **2020**, 1212, 128129	3.4	15
155	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
154	Vibrational and UV spectra, first order hyperpolarizability, NBO and HOMO-LUMO analysis of 4-chloro-N-(2-methyl-2,3-dihydroindol-1-yl)-3-sulfamoyl-benzamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 122, 1-14	4.4	15
153	Quantum mechanical study of the structure and spectroscopic, first order hyperpolarizability, Fukui function, NBO, normal coordinate analysis of phenyl-N-(4-methyl phenyl) nitrone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 112, 62-77	4.4	15
152	FTIR, FT-RAMAN, NMR, spectra, normal co-ordinate analysis, NBO, NLO and DFT calculation of N,N-diethyl-4-methylpiperazine-1-carboxamide molecule. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 275-86	4.4	15
151	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

150	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
149	Study of vibrational spectra, normal coordinate analysis and molecular structure of 6-(2,3-dichlorophenyl)-1,2,4-triazine-3,5-diamine using density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 121, 420-9	4.4	13
148	Quantum chemical studies, vibrational analysis, molecular structure, first order hyper polarizability, NBO and HOMO-LUMO analysis of 3-hydroxybenzaldehyde and its cation. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 789-99	4.4	13
147	An experimental and theoretical study of the vibrational spectra and structure of Isosorbide dinitrate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 109, 322-30	4.4	13
146	Normal coordinate analysis and vibrational spectroscopy (FT-IR and FT-Raman) studies of (2S)-2-amino-3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid using ab initio HF and DFT method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2012**, 99, 90-6	4.4	13
145	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
144	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
143	Vibrational spectroscopy investigation using ab initio and DFT vibrational analysis of 7-chloro-2-methylamino-5-phenyl-3H-1,4-benzodiazepine-4-oxide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 113, 224-35	4.4	12
142	Optical, vibrational (FT-IR and FT-Raman), electronic and molecular docking investigations of 1 Phenyl Isatin. *Optik*, **2019**, 182, 1211-1227	2.5	11
141	QM/MM methodology, docking and spectroscopic (FT-IR/FT-Raman, NMR, UV) and Fukui function analysis on adrenergic agonist. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 137, 841-55	4.4	11
140	Growth and characterization of l -Serine: A promising acentric organic crystal. *Physica B: Condensed Matter*, **2018**, 541, 32-42	2.8	11
139	Spectroscopic studies, potential energy surface and molecular orbital calculations of pramipexole. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 64-73	4.4	11
138	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
137	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
136	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
135	Synthesis, molecular structure, spectral investigation on (E)-1-(4-bromophenyl)-3-(4-(dimethylamino)phenyl)prop-2-en-1-one. *Journal of Molecular Structure*, **2016**, 1103, 145-155	3.4	10
134	Spectroscopic (FT-IR, FT-Raman), first order hyperpolarizabilities, NBO, Fukui function and molecular docking study of N-(4-Chloro-3-methylphenyl)-2-phenylacetamide. *Optik*, **2017**, 140, 1127-1142	2.5	10
133	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

132	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
131	Vibrational spectra of 3,5-diamino-6-chloro-N-(diaminomethylene) pyrazine-2-carboxamide: combined experimental and theoretical studies. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 127, 157-67	4.4	10
130	Molecular structure analysis and spectroscopic characterization of 5-ethyl-5-phenyl-1,3-diazinane-4,6-dione with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 106, 310-20	4.4	10
129	Quantum mechanical study of the structure and spectroscopic (FT-IR, FT-Raman), first-order hyperpolarizability, NBO and HOMO-LUMO analysis of S-S-2 methylamino-1-phenyl propan-1-ol. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 107, 386-98	4.4	10
128	Experimental and theoretical investigations of spectroscopic properties of 8-chloro-1-methyl-6-phenyl-4H-[1,2,4]triazolo[4,3-a][1,4]benzodiazepine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 106, 129-45	4.4	10
127	Vibrational and spectroscopic investigation on the structure of 5H-dibenzo[b,f]azipine-5-carboxamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 114, 1-10	4.4	10
126	Vibrational spectroscopy investigation using density functional theory on 7-chloro-3-methyl-2H-1,2,4- benzothiadiazine 1,1-dioxide. *Journal of Raman Spectroscopy*, **2009**, 40, 639-644	2.3	10
125	Molecular orbital studies (hardness, chemical potential, electronegativity and electrophilicity), vibrational spectroscopic investigation and normal coordinate analysis of 5-{1-hydroxy-2-[(propan-2-yl)amino]ethyl}benzene-1,3-diol. *Spectrochimica Acta - Part A: Molecular*	4.4	9
124	Quantum mechanical study of the structure and spectroscopic (FTIR, FT-Raman), first-order hyperpolarizability and NBO analysis of 1,2-benzoxazol-3-ylmenthane sulfonamide. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 128, 603-13	4.4	9
123	Comprehensive spectroscopic (FT-IR, FT-Raman, 1H and 13C NMR) identification and computational studies on 1-acetyl-1H-indole-2,3-dione. *Open Chemistry*, **2017**, 15, 225-237	1.6	9
122	Normal coordinate analysis, molecular structure, vibrational and electronic spectral investigation of 7-(1,3-dioxolan-2-ylmethyl)-1,3-dimethylpurine-2,6-dione by ab initio HF and DFT method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 118, 578-88	4.4	9
121	Synthesis, spectroscopic (FT-IR, FT-Raman, 13C, 1H, UV) study, first order hyperpolarizability, NBO analysis, HOMO and LUMO analysis of 2(2-Hydroxyphenyl)-N-(4-Methylphenyl) Nitrone. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 109, 272-81	4.4	9
120	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
119	Vibrational spectra and Wavefunction investigation for antidepressant drug of Amoxapine based on quantum computational studies. *Chemical Data Collections*, **2021**, 33, 100699	2.1	9
118	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
117	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
116	Structural investigation, spectroscopic and energy level studies of Schiff base: 2-[(3?- N -salicylidenephenyl)benzimidazole] using experimental and DFT methods. *Journal of Molecular Structure*, **2017**, 1139, 247-254	3.4	8
115	A computational and spectroscopic interpretation (FT-IR, FT-Raman, UV–vis 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

114	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
113	Molecular structure, vibrational spectra, NBO, Fukui function, HOMO-LUMO analysis and molecular docking study of 6-[(2-methylphenyl)sulfanyl]-5-propylpyrimidine-2,4(1H,3H)-dione. *Macedonian Journal of Chemistry and Chemical Engineering*, **2017**, 36,	1.1	8
112	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
111	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
110	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
109	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
108	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
107	Growth, structural and characterization of a novel third order nonlinear optical Benzimidazolium Maleate single crystal. *Journal of Molecular Structure*, **2017**, 1146, 5-13	3.4	7
106	Spectroscopic studies (FT-IR, FT-Raman, UV-Visible), normal co-ordinate analysis, first-order hyperpolarizability and HOMO, LUMO studies of 3,4-dichlorobenzophenone by using Density Functional Methods. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 151, 644-54	4.4	7
105	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
104	Quantum mechanical computation, spectroscopic exploration and molecular docking analysis of 2-Bromo-4-fluoroacetanilide. *Journal of Molecular Structure*, **2020**, 1220, 128639	3.4	7
103	Experimental and computational study on molecular structure and vibrational analysis of 4,5-Bis(hydroxymethyl)-2-methylpyridin-3-ol by normal coordinate treatment. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 191-201	4.4	7
102	Spectroscopic (FT-IR, FT-Raman, UV□isible) and quantum chemical studies of 4-Chloro-3-iodobenzophenone. *Journal of Molecular Structure*, **2017**, 1128, 685-693	3.4	7
101	Density functional theory and Ab initio studies of vibrational spectroscopic (FT-IR, FT-Raman and UV) first order hyperpolarizabilities, NBO, HOMO□UMO and TD-DFT analysis of the 1,2-Dihydropyrazolo (4,3-E) Pyrimidin-4-one. *Solid State Sciences*, **2013**, 16, 45-52	3.4	7
100	Density functional theory and ab initio studies of vibrational spectra of 2-bis (2-chloroethyl) aminoperhydro-1,3,2-oxazaphosphorinane-2-oxide. *Molecular Simulation*, **2011**, 37, 1276-1288	2	7
99	Vibrational spectral assignments of paraldehyde by ab initio and density functional methods. *Journal of Molecular Modeling*, **2008**, 14, 375-83	2	7
98	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
97	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

96	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
95	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
94	The spectroscopic (FT-IR, FT-Raman and NMR), NCA, Fukui function analysis first order hyperpolarizability, TGA of 6-chloro-3,4dihydro-2H-1,2,4-benzothiazine-7-sulphonamide1,1-dioxide by ab initio HF and Density Functional method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 123, 230-40	4.4	6
93	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
92	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
91	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
90	Vibrational spectra, first order hyperpolarizability, NBO, Fukui function and HOMO-LUMO analysis of 2-[4-(1,3-benzodioxol-5-ylmethyl)-1-piperazinyl] pyrimidine. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 115, 654-66	4.4	5
89	Experimental spectroscopic (FTIR, FT-Raman, FT-NMR, UV-Visible) and DFT studies of 1-ethyl-1,4-dihydro-7-methyl-4oxo-1,8 napthyridine-3-carboxylic acids. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2013**, 116, 220-35	4.4	5
88	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
87	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
86	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
85	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
84	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
83	Anti-microbial activity, molecular profiling, electronic properties and molecular docking investigations of 5-[1-hydroxy-2-(isopropylamino)ethyl] benzene-1,3-diol. *Journal of Molecular Structure*, **2022**, 1247, 131299	3.4	5
82	Scaled Quantum Chemical Studies of the Molecular Structure and Vibrational Spectra of Minoxidil. *Spectroscopy Letters*, **2015**, 48, 63-73	1.1	4
81	DFT electronic structure calculations, spectroscopic studies, and normal coordinate analysis of 2-[(5-nitro-1,3-thiazol-2-yl)carbamoyl]phenyl acetate. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 138, 743-52	4.4	4
80	Molecular docking, spectroscopic studies and quantum calculations on nootropic drug. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 123, 503-10	4.4	4
79	Normal coordinate analysis and vibrational spectroscopy (FT-IR and FT-Raman) studies of 5-methyl-N-[4-(trifluoromethyl) phenyl]-isoxazole-4-carboxamide using density functional method. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2014**, 132, 142-51	4.4	4

78	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
77	Vibrational spectroscopy, quantum computational and molecular docking studies on 2-chloroquinoline-3-carboxaldehyde. *Heliyon*, **2021**, 7, e07529	3.6	4
76	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
75	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
74	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
73	Vibrational Assignments, First-Order Hyperpolarizability and Molecular Structure of 5-(2-Chlorphenyl)-7-nitro-2,3-dihydro-1,4-benzodiazepine-2-one by Hartree-Fock and Density Functional Theory Calculations. *Asian Journal of Chemistry*, **2013**, 25, 6771-6776	0.4	3
72	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
71	Structural and spectroscopic characterization oF N[(1E)-(4-fluorophenyl)methylidene]thiophene-2-carbohydrazide, a potential precursor to bioactive agents. *Macedonian Journal of Chemistry and Chemical Engineering*, **2016**, 35, 63	1.1	3
70	Synthesis, spectroscopic elucidation (FT-IR, FT-Raman, UV–Vis), electronic properties and biological activities (antimicrobial, docking) of semicarbazide derivative. *Materials Today: Proceedings*, **2020**, 50, 2847-2847	1.4	3
69	IN SILICO DRUG EVALUATION AND DRUG RESEARCH OF BIOACTIVE MOLECULE METHYL 4-BROMO-2-FLUOROBENZOATE. *Ankara Universitesi Eczacilik Fakultesi Dergisi*,10-10	0	3
68	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
67	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
66	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
65	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*	1	3
64	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
63	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
62	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
61	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

60	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
59	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
58	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
57	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
56	Spectroscopic, quantum chemical calculations, and molecular docking analysis of 3-Chlorophenyl boronic acid. *Spectroscopy Letters*, **2020**, 53, 778-792	1.1	2
55	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
54	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
53	Structural, spectral, electronic and optical investigations of D-(-)-alpha-Phenylglycine: protease kinase inhibitor. *Spectroscopy Letters*,1-17	1.1	2
52	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
51	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
50	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
49	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
48	Normal co-ordinate analysis, molecular structural, non-linear optical, second order perturbation studies of Tizanidine by density functional theory. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2015**, 139, 189-99	4.4	1
47	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
46	Theoretical and experimental spectroscopic studies of monomeric and dimeric structures of 4-hydroxybenzamide. *Journal of Molecular Structure*, **2020**, 1206, 127742	3.4	1
45	Molecular Structure, Vibrational Spectroscopy and Homo, Lumo Studies of 4-methyl-N-(2-methylphenyl) Benzene Sulfonamide Using DFT Method. *Advanced Materials Research*, **2013**, 665, 101-111	0.5	1
44	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
43	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

42	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
41	Structural, spectral elucidation, wavefunctional properties, natural bond orbitals, and molecular docking analysis of synthesized 1-phenyl-3(4-methoxyphenyl)-2-propenone: protease kinase inhibitor. *Spectroscopy Letters*,1-17	1.1	1
40	Structural examination, theoretical calculations, and pharmaceutical scanning of a new tetralone based chalcone derivative. *Journal of Molecular Structure*, **2022**, 1253, 132296	3.4	1
39	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
38	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
37	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
36	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
35	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
34	Quantum Chemical, Vibrational Spectroscopic and Molecular Docking Studies of 1-(Diphenylmethyl)Piperazine. *Polycyclic Aromatic Compounds*, **2020**, 1-21	1.3	1
33	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
32	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
31	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
30	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
29	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
28	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
27	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
26	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
25	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

24	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
23	Experimental Spectroscopic, Quantum Computational, Hirshfeld Surface, Molecular Docking, and Electronic Excitation Studies on an Antibiotic Agent: SDZ. *Polycyclic Aromatic Compounds*,1-25	1.3	1
22	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
21	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
20	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
19	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
18	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
17	Growth, spectral, optical, electrical and computational analysis of sodium oxalate single crystals. *Heliyon*, **2021**, 7, e06527	3.6	0
16	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
15	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
14	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
13	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
12	Computational investigation, effects of polar and non-polar solvents on optimized structure with topological parameters (ELF, LOL, AIM, and RDG) of three glycine derivative compounds. *Structural Chemistry*,1	1.8	0
11	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
10	Structural, optical, thermal and NLO behavior of zinc hydrogen maleate dihydrate single crystal. *Materials Science-Poland*, **2017**, 35, 773-784	0.6	
9	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	
8	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	
7	Spectroscopic, quantum computational, molecular docking and biological parameters of 4-phenylbutyrophenone: a neuroleptic agent. *Chemical Papers*, **2021**, 75, 3931-3948	1.9	

6	STRUCTURAL AND PHARMACEUTICAL EVALUATION OF 4-HYDROXY-BENZAMIDE DERIVATIVE: ANTI-BACTERIAL AND ANTI-VIRAL POTENT. *Ankara Universitesi Eczacilik Fakultesi Dergisi*,467-479	0
5	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
4	Molecular Structure, Spectroscopic Assessment, PDOS, Topology Evaluation and Docking Studies of 2-Chloro-5-nitrobenzophenone. *Analytical Chemistry Letters*, **2022**, 12, 198-220	1
3	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
2	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
1	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	