

# Shabbir Ahmad

## List of Publications by Year in descending order

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35  
papers

719  
citations

471509

17  
h-index

580821

25  
g-index

35  
all docs

35  
docs citations

35  
times ranked

704  
citing authors

#	ARTICLE	IF	CITATIONS
1	Anharmonic vibrational studies of l-aspartic acid using HF and DFT calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 96, 992-1004.	3.9	54
2	DFT/B3LYP calculations, in vitro cytotoxicity and antioxidant activities of steroidal pyrimidines and their interaction with HSA using molecular docking and multispectroscopic techniques. <i>Bioorganic Chemistry</i> , 2017, 73, 83-99.	4.1	50
3	FTIR, FT-Raman, UV-Vis spectra and quantum chemical calculations of allantoin molecule and its hydrogen bonded dimers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 961-978.	3.9	49
4	Spectroscopic (FTIR, FT-Raman, <sup>1</sup> H NMR and UV-Vis) and DFT/TD-DFT studies on cholesteno [4,6-b,c]-2,5-dihydro-1,5-benzothiazepine. <i>Journal of Molecular Structure</i> , 2019, 1178, 570-582.	3.6	48
5	Molecular structure, anharmonic vibrational analysis and electronic spectra of o-, m-, p-iodonitrobenzene using DFT calculations. <i>Journal of Molecular Structure</i> , 2014, 1059, 239-254.	3.6	39
6	Quantum chemical and spectroscopic investigations of 3-methyladenine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 128, 653-664.	3.9	39
7	Synthesis, spectroscopic, computational (DFT/B3LYP), AChE inhibition and antioxidant studies of imidazole derivative. <i>Journal of Molecular Structure</i> , 2018, 1151, 327-342.	3.6	38
8	FT-IR and FT-Raman spectra, MEP and HOMO-LUMO of 2,5-dichlorobenzonitrile: DFT study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 136, 464-472.	3.9	29
9	Structural, vibrational and electronic absorption characteristics of the monohydrate organic salt of 2-amino-5-bromo-6-methyl-4-pyrimidinol and 2,3-pyrazinedicarboxylic acid: A combined experimental and computational study. <i>Journal of Molecular Structure</i> , 2019, 1177, 229-241.	3.6	25
10	Computational studies of vibrational spectra and molecular properties of 6-methyluracil using HF, DFT and MP2 methods. <i>Indian Journal of Physics</i> , 2011, 85, 239-260.	1.8	24
11	Structural elucidation, density functional calculations and contribution of intermolecular interactions in cholest-4-en-3-one crystals: Insights from X-ray and Hirshfeld surface analysis. <i>Journal of Molecular Structure</i> , 2015, 1084, 274-283.	3.6	23
12	Quantum chemical calculations and analysis of FTIR, FT-Raman and UV-Vis spectra of temozolomide molecule. <i>Journal of Molecular Structure</i> , 2015, 1099, 453-462.	3.6	22
13	Experimental and computational investigation of novel dihydrated organic single crystal of 2,4,6-triaminopyrimidine and 3,5-dinitrobenzoic acid: Linear and nonlinear optical response with limiting performance. <i>Journal of Solid State Chemistry</i> , 2021, 300, 122255.	2.9	22
14	Computational and anti-tumor studies of 7a-Aza-B-homostigmast-5-eno [7a, 7-d] tetrazole-3-yl chloride. <i>Journal of Molecular Structure</i> , 2016, 1108, 411-426.	3.6	21
15	DFT/TD-DFT calculations, spectroscopic characterizations (FTIR, NMR, UV-Vis), molecular docking and enzyme inhibition study of 7-benzoyloxycoumarin. <i>Computational Biology and Chemistry</i> , 2018, 73, 65-78.	2.3	21
16	DFT, Hirshfeld surfaces, spectral and in vivo cytotoxic studies of 7a-Aza-B-homostigmast-5-eno [7a,7-d] tetrazole. <i>Journal of Molecular Structure</i> , 2015, 1099, 588-600.	3.6	20
17	Synthesis, X-ray crystallography, spectroscopic (FT-IR, <sup>1</sup> H & <sup>13</sup> C NMR and UV), computational (DFT/B3LYP) and enzymes inhibitory studies of 7-hydroximincholest-5-en-3-ol acetate. <i>Journal of Molecular Structure</i> , 2016, 1116, 317-332.	3.6	17
18	Growth, structure, Hirshfeld surface and spectroscopic properties of 2-amino-4-hydroxy-6-methylpyrimidinium-2,3-pyrazinedicorboxylate single crystal. <i>Journal of Molecular Structure</i> , 2018, 1155, 695-710.	3.6	17

#	ARTICLE	IF	CITATIONS
19	Anharmonic vibrational and electronic spectral study of 2-amino-4-hydroxy-6-methylpyrimidine: A combined experimental (FTIR, FT-Raman, UV-Vis) and theoretical (DFT, MP2) approach. <i>Journal of Molecular Structure</i> , 2017, 1148, 89-100.	3.6	16
20	Cocrystallization of 2,3-dimethylquinoxaline with 3,5-dinitrobenzoic acid: Crystal structure, Hirshfeld surface, spectroscopic features and DFT studies. <i>Journal of Molecular Structure</i> , 2019, 1198, 126894.	3.6	16
21	FTIR, FT-Raman and UV-Vis spectral studies of d-tyrosine molecule. <i>Journal of Molecular Structure</i> , 2016, 1105, 169-177.	3.6	15
22	Experimental vibrational spectroscopy (FTIR and FT-Raman) of D-tryptophan and its anharmonic theoretical studies using density functional theory. <i>Journal of Molecular Structure</i> , 2018, 1171, 315-322.	3.6	14
23	Anharmonic vibrational spectroscopy and investigation of intramolecular mode couplings in adenine. <i>Vibrational Spectroscopy</i> , 2011, 56, 51-59.	2.2	12
24	Study of molecular structure, anharmonic vibrational dynamic and electronic properties of sulindac using spectroscopic techniques integrated with quantum chemical calculations. <i>Journal of Molecular Structure</i> , 2017, 1147, 603-615.	3.6	11
25	Intramolecular charge transfer-based linear and nonlinear optical properties of a D-π-A-D type organic chromophore: Experimental and computational approach. <i>Journal of Nonlinear Optical Physics and Materials</i> , 2022, 31, .	1.8	11
26	Approximate solution of the mode-mode coupling integral: Application to cytosine and its deuterated derivative. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2010, 77, 446-456.	3.9	10
27	Anharmonic vibrational analysis of uracil by ab initio Hartree-Fock and density functional theory calculations. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 18-20.	1.5	9
28	Vibrational and electronic spectral analysis of 2,3-pyrazinedicarboxylic acid: A combined experimental and theoretical study. <i>Spectroscopy Letters</i> , 2016, 49, 449-457.	1.0	9
29	Anharmonic vibrational spectra and mode-mode couplings analysis of 2-aminopyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 188, 26-31.	3.9	9
30	Experimental thermophysical properties and DFT calculations of imidazolium ionic liquids and 2-butanol mixtures. <i>Fluid Phase Equilibria</i> , 2020, 508, 112447.	2.5	9
31	Electron impact ionisation cross section for organoplatinum compounds. <i>Molecular Physics</i> , 2016, 114, 3104-3111.	1.7	6
32	Detailed molecular, structural and spectral studies of bimetallic salt, [Ni(L)][CoCl <sub>4</sub> ] where L=3,7-bis(2-aminoethyl)-1,3,5,7-tetraazabicyclo(3.3.1)nonane. <i>Journal of Molecular Structure</i> , 2017, 1138, 90-101.	3.6	6
33	FTIR and FT-Raman spectra of 6-(dimethylamino)purine and its theoretical studies of anharmonic vibrational analysis using quantum chemical calculations. <i>Vibrational Spectroscopy</i> , 2021, 113, 103224.	2.2	5
34	Quantum chemical and spectroscopic investigations of 4-Hydroxy-7-methyl-1,8-naphthyridine-3-carboxylic acid. <i>Journal of Theoretical and Computational Chemistry</i> , 2016, 15, 1650042.	1.8	3
35	3 <sup>β</sup> -Acetoxy cholest-5-ene crystals: Catalytic synthesis, structural elucidation, contribution of intermolecular interactions and density functional theory calculations. <i>Journal of Molecular Structure</i> , 2020, 1221, 128833.	3.6	0