Anubha Srivastava

List of Publications by Year
in descending order

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40	696	516710 16	580821 25
papers	citations	h-index	g-index

40	40	40	746
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Vibrational analysis and chemical activity of paracetamolâ€“oxalic acid cocrystal based on monomer and dimer calculations: DFT and AIM approach. RSC Advances, 2016, 6, 10024-10037.	3.6	60
2	Molecular structure, spectral analysis and hydrogen bonding analysis of ampicillin trihydrate: a combined DFT and AIM approach. New Journal of Chemistry, 2015, 39, 9800-9812.	2.8	53
3	Vibrational spectroscopic, NBO, AIM, and multiwfn study of tectorigenin: A DFT approach. Journal of Molecular Structure, 2020, 1217, 128443.	3.6	43
4	A computational study on conformational geometries, chemical reactivity and inhibitor property of an alkaloid bicuculline with Î³-aminobutyric acid (GABA) by DFT. Computational and Theoretical Chemistry, 2012, 993, 80-89.	2.5	41
5	Conformational analysis and vibrational study of daidzein by using FT-IR and FT-Raman spectroscopies and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 405-415.	3.9	37
6	Studies of molecular structure, hydrogen bonding and chemical activity of a nitrofurantoin-<scp>l</scp>-proline cocrystal: a combined spectroscopic and quantum chemical approach. RSC Advances, 2016, 6, 74135-74154.	3.6	37
7	Molecular structure, spectral investigation (1H NMR, 13C NMR, UVâ€“Visible, FT-IR, FT-Raman), NBO, intramolecular hydrogen bonding, chemical reactivity and first hyperpolarizability analysis of formononetin [7-hydroxy-3(4-methoxyphenyl)chromone]: A quantum chemical study. Journal of Molecular Structure, 2015, 1084, 55-73.	3.6	36
8	Computational evaluation on molecular stability, reactivity, and drug potential of frovatriptan from DFT and molecular docking approach. Computational and Theoretical Chemistry, 2020, 1191, 113031.	2.5	31
9	Solid state characterization of an antioxidant alkaloid boldine using vibrational spectroscopy and quantum chemical calculations. Vibrational Spectroscopy, 2011, 56, 82-88.	2.2	22
10	Antagonistic properties of a natural product â€“ Bicuculline with the gamma-aminobutyric acid receptor: Studied through electrostatic potential mapping, electronic and vibrational spectra using ab initio and density functional theory. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 84, 144-155.	3.9	22
11	Structural, electronic, thermodynamical and charge transfer properties of Chloramphenicol Palmitate using vibrational spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 101, 335-342.	3.9	22
12	Molecular structure and vibrational spectroscopic analysis of an antiplatelet drug; clopidogrel hydrogen sulphate (form 2) â€“ A combined experimental and quantum chemical approach. Journal of Molecular Structure, 2010, 964, 88-96.	3.6	19
13	Molecular structure, vibrational spectra and HOMO, LUMO analysis of yohimbine hydrochloride by density functional theory and ab initio Hartreeâ€“Fock calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2011, 82, 270-278.	3.9	19
14	Study of molecular structure, vibrational, electronic and NMR spectra of oncocalyxone A using DFT and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 367-377.	3.9	19
15	A comparative computational study on molecular structure, NBO analysis, multiple interactions, chemical reactivity and first hyperpolarisability of imatinib mesylate polymorphs using DFT and QTAIM approach. Molecular Simulation, 2014, 40, 1099-1112.	2.0	18
16	Study of polymorphism in imatinib mesylate: A quantum chemical approach using electronic and vibrational spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 103, 325-332.	3.9	16
17	Quantum chemical and experimental studies on the structure and vibrational spectra of efavirenz. Vibrational Spectroscopy, 2010, 53, 112-116.	2.2	15
18	A computational study on molecular structure, multiple interactions, chemical reactivity and molecular docking studies on 6[D (â^') Î±-amino-phenyl-acetamido] penicillanic acidÂ(ampicillin). Molecular Simulation, 2016, 42, 863-873.	2.0	13

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19	Molecular Structure, Spectral Investigations, Hydrogen Bonding Interactions and Reactivity-Property Relationship of Caffeine-Citric Acid Cocrystal by Experimental and DFT Approach. Frontiers in Chemistry, 2021, 9, 708538.	3.6	13
20	Combined spectroscopic and quantum chemical studies of ezetimibe. Journal of Molecular Structure, 2016, 1125, 193-203.	3.6	12
21	Non-covalent interactions and spectroscopic study of chalcone derivative 1-(4-chlorophenyl)-3-(5-methylfuran-2-yl) prop-2-en-1-one. Journal of Molecular Structure, 2020, 1201, 127145.	3.6	12
22	FT-Raman, FT-IR, UV spectroscopic, NBO and DFT quantum chemical study on the molecular structure, vibrational and electronic transitions of clopidogrel hydrogen sulfate form 1: A comparison to form 2. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 104, 409-418.	3.9	11
23	Spectroscopic, quantum chemical calculation and molecular docking of dipfluzine. Journal of Molecular Structure, 2016, 1125, 751-762.	3.6	11
24	Spectroscopic and molecular structure (monomeric and dimeric model) investigation of Febuxostat: A combined experimental and theoretical study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 1-12.	3.9	11
25	Study of molecular structure and hydrogen bond interactions in dipfluzine-benzoic acid (DIP-BEN) cocrystal using spectroscopic and quantum chemical method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 216, 7-14.	3.9	11
26	Spectroscopic (far or terahertz, mid-infrared and Raman) investigation, thermal analysis and biological activity of piplartine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 184, 368-381.	3.9	10
27	Characterization and intramolecular bonding patterns of busulfan: Experimental and quantum chemical approach. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 390-399.	3.9	10
28	Vibrational spectra, hydrogen bonding interactions and chemical reactivity analysis of nicotinamideâ€“citric acid cocrystals by an experimental and theoretical approach. New Journal of Chemistry, 2019, 43, 15956-15967.	2.8	10
29	A novel approach to design febuxostat-salicylic acid eutectic system: evaluation and characterization. CrystEngComm, 2019, 21, 310-320.	2.6	10
30	Spectroscopic and quantum chemical study of an alkaloid aristolochic acid I. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 258-269.	3.9	9
31	Quantum chemical and experimental studies on the structure and vibrational spectra of an alkaloidâ€“Corlumine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 118, 470-480.	3.9	9
32	Experimental and Quantum Chemical Studies of Nicotinamide-Oxalic Acid Salt: Hydrogen Bonding, AIM and NBO Analysis. Frontiers in Chemistry, 2022, 10, 855132.	3.6	7
33	Study of hydrogen-bonding, vibrational dynamics and structure-activity relationship of genistein using spectroscopic techniques coupled with DFT. Journal of Molecular Structure, 2017, 1130, 929-939.	3.6	6
34	Study of conformational stability, structural, electronic and charge transfer properties of cladrin using vibrational spectroscopy and DFT calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 615-628.	3.9	5
35	A combined experimental (IR, Raman and UVâ€“Vis) and quantum chemical study of canadine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 191, 249-258.	3.9	4
36	Spectroscopic and quantum chemical analysis of a natural product â€“ Hayatin hydrochloride. Journal of Molecular Structure, 2015, 1093, 101-112.	3.6	3

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37	Structural insights, protein-ligand interactions and spectroscopic characterization of isoformononetin. Journal of Molecular Structure, 2017, 1133, 479-491.	3.6	3
38	Evaluation of efficacy of Valsalva for attenuating needle puncture pain in first time nonremunerated voluntary plateletpheresis donors: A prospective, randomized controlled trial. Asian Journal of Transfusion Science, 2021, 15, 68.	0.3	3
39	Structural properties of a novel heterocyclic chalcones derivative, (E)-3-(5-methyl furan-2-yl)-1-phenyl propâ€2-en-1-one: A spectroscopic and DFT perception. Journal of Molecular Structure, 2021, 1244, 130973.	3.6	2
40	Thromboelastography as a tool for quality check of apheresis platelets. Asian Journal of Transfusion Science, 2016, 10, 111.	0.3	1