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	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
2	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
3	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
4	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
5	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
6	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
7	Vibrational spectroscopic, NBO, AIM, and multiwfn study of tectorigenin: A DFT approach. Journal of Molecular Structure, 2020, 1217, 128443.	3.6	43
8	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
9	A novel approach to design febuxostat-salicylic acid eutectic system: evaluation and characterization. CrystEngComm, 2019, 21, 310-320.	2.6	10
10	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
11	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
12	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
13	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
14	Structural insights, protein-ligand interactions and spectroscopic characterization of isoformononetin. Journal of Molecular Structure, 2017, 1133, 479-491.	3.6	3
15	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
16	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
17	Combined spectroscopic and quantum chemical studies of ezetimibe. Journal of Molecular Structure, 2016, 1125, 193-203.	3.6	12
18	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

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19	Spectroscopic, quantum chemical calculation and molecular docking of dipfluzine. Journal of Molecular Structure, 2016, 1125, 751-762.	3.6	11
20	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
21	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
22	Thromboelastography as a tool for quality check of apheresis platelets. Asian Journal of Transfusion Science, 2016, 10, 111.	0.3	1
23	Spectroscopic and quantum chemical analysis of a natural product â€“ Hayatin hydrochloride. Journal of Molecular Structure, 2015, 1093, 101-112.	3.6	3
24	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
25	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
26	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
27	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
28	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
29	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
30	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
31	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
32	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
33	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
34	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
35	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
36	Solid state characterization of an antioxidant alkaloid boldine using vibrational spectroscopy and quantum chemical calculations. Vibrational Spectroscopy, 2011, 56, 82-88.	2.2	22

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37	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
38	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
39	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
40	Quantum chemical and experimental studies on the structure and vibrational spectra of efavirenz. Vibrational Spectroscopy, 2010, 53, 112-116.	2.2	15