Leena Sinha

List of Publications by Year
in descending order

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50	983	471509	454955
papers	citations	17	30
		h-index	g-index

50	50	50	1028
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Spectroscopic, electronic structure, molecular docking, and molecular dynamics simulation study of 7-Trifluoromethyl-1H-indole-2-carboxylic acid as an aromatase inhibitor. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2022, 280, 121530.	3.9	3
2	Thermoacoustic and DFT Analysis of N,N-Dimethylacetamide (DMA) with 1-Propanol and Methanol at 293.15, 303.15, and 313.15ÂK. Brazilian Journal of Physics, 2021, 51, 515-526.	1.4	4
3	Surface modification and characterization of h-BN-doped PVP thin film and its application as humidity sensor with theoretical DFT calculations. Chemical Papers, 2021, 75, 4055-4068.	2.2	9
4	Study of molecular association in binary mixtures of poly(vinyl pyrrolidone) (PVP) with ethanol, 1-propanol and 1-butanol through thermo-acoustical, FT-IR, UVâ€“Vis spectroscopy and DFT studies. European Physical Journal D, 2021, 75, 1.	1.3	1
5	Thermodynamic, spectroscopic and DFT studies of binary mixtures of poly(vinylpyrrolidone) (PVP) with ethanol, 1-propanol and 1-butanol. Journal of Molecular Liquids, 2020, 299, 112237.	4.9	10
6	DFT Study on the Electronic Properties, Spectroscopic Profile, and Biological Activity of 2-Amino-5-trifluoromethyl-1,3,4-thiadiazole with Anticancer Properties. ACS Omega, 2020, 5, 30073-30087.	3.5	17
7	Experimental and theoretical DFT (B3LYP, X3LYP, CAM-B3LYP and M06-2X) study on electronic structure, spectral features, hydrogen bonding and solvent effects of 4-methylthiadiazole-5-carboxylic acid. Molecular Simulation, 2019, 45, 1029-1043.	2.0	33
8	Virtual screening in drug-likeness and structure/activity relationship of pyridazine derivatives as Anti-Alzheimer drugs. Journal of King Saud University - Science, 2019, 31, 595-601.	3.5	41
9	A combined experimental and theoretical DFT (B3LYP, CAM-B3LYP and M06-2X) study on electronic structure, hydrogen bonding, solvent effects and spectral features of methyl 1H-indol-5-carboxylate. Journal of Molecular Structure, 2017, 1137, 725-741.	3.6	47
10	First principle study of a potential bioactive molecule with tetrahydroisoquinoline, carbothiomide and adamantane scaffolds. Journal of Molecular Structure, 2017, 1143, 204-216.	3.6	3
11	Spectroscopic and electronic structure calculation of a potential antibacterial agent incorporating pyrido-dipyrimidine-dione moiety using first principles. Journal of Molecular Structure, 2016, 1110, 128-137.	3.6	8
12	Prediction of molecular properties and spectroscopic profile of Riluzole with different functionals (B3LYP, M06-2X, MPWLYP): A combined theoretical and experimental study. Journal of Molecular Structure, 2016, 1106, 265-276.	3.6	7
13	Conformational search, spectral analysis and electronic properties of 5-(4-Pyridinyl)-1,3,4-thiadiazol-2-amine. Journal of Molecular Structure, 2016, 1108, 112-125.	3.6	5
14	Investigations on Molecular Structure, Electronic Properties, NLO Properties and Comparison of Drug-Likeness of Triazolothiadiazole Derivatives by Quantum Methods and QSAR Analysis. Reviews in Theoretical Science, 2016, 4, 85-96.	0.5	5
15	Development of certain novel N-(2-(2-(2-oxoindolin-3-ylidene)hydrazinecarbonyl)phenyl)-benzamides and 3-(2-oxoindolin-3-ylideneamino)-2-substituted quinazolin-4(3H)-ones as CFM-1 analogs: Design, synthesis, QSAR analysis and anticancer activity. European Journal of Medicinal Chemistry, 2015, 92, 191-201.	5.5	30
16	A Combined theoretical and experimental study of conformational and spectroscopic profile of 2-acetamido-5-aminopyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 143, 147-157.	3.9	7
17	Conformational and spectroscopic behaviors of 2,4-xylyl isothiocyanate. Journal of Molecular Structure, 2015, 1087, 113-120.	3.6	3
18	FT-IR and FT-Raman spectroscopic signatures, vibrational assignments, NBO, NLO analysis and molecular docking study of 2-{[5-(adamantan-1-yl)-4-methyl-4H-1,2,4-triazol-3-yl]sulfanyl}-N,N-dimethylethanamine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 140, 1-14.	3.9	15

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19	Exploring QSARs of some benzenesulfonamides incorporating cyanoacrylamide moieties as a carbonic anhydrase inhibitors (specifically against tumor-associated isoforms IX and XII). Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 519-523.	5.2	8
20	Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid. Journal of Molecular Structure, 2015, 1095, 100-111.	3.6	5
21	Study on molecular structure, spectroscopic behavior, NBO, and NLO analysis of 3-methylbezothiazole-2-thione. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 146, 129-141.	3.9	15
22	Spectroscopic and electronic structure calculation of a potential chemotherapeutic agent 5-propyl-6-(p-tolylsulfanyl)pyrimidine-2,4(1H,3H)-dione using first principles. Journal of Molecular Structure, 2015, 1100, 225-236.	3.6	5
23	Structure Activity Relationship and Quantitative Structure-Activity Relationships Modeling of Antitrypanosomal Activities of Alkyldiamine Cryptolepine Derivatives. Journal of Computational and Theoretical Nanoscience, 2015, 12, 2421-2427.	0.4	7
24	Syntheses, structural elucidation, thermal properties, theoretical quantum chemical studies (DFT) and biological studies of barbituricâ€“hydrazone complexes. Journal of Saudi Chemical Society, 2015, 19, 217-226.	5.2	14
25	Experimental (FT-IR, FT-Raman, UV and NMR) and quantum chemical studies on molecular structure, spectroscopic analysis, NLO, NBO and reactivity descriptors of 3,5-Difluoroaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 135, 283-295.	3.9	54
26	Structural and spectroscopic characterization of a novel potential anti-inflammatory agent 3-(adamantan-1-yl)-4-ethyl-1H-1,2,4-triazole-5(4H)thione by first principle calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 124, 108-123.	3.9	17
27	Molecular structure, vibrational and electronic properties of 4-Phenyl-3H-1,3-thiazol-2-ol using density functional theory and comparison of drug efficacy of keto and enol forms by QSAR analysis. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 132, 568-581.	3.9	6
28	Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 126-136.	3.9	14
29	Structural, spectroscopic (FT-IR, FT-Raman and UV) studies, HOMOâ€“LUMO, NBO, NLO analysis and reactivity descriptors of 2,3 Difluoroaniline and 2,4-Difluoroaniline. Journal of Molecular Structure, 2014, 1074, 457-466.	3.6	21
30	A combined experimental and theoretical investigation of 2-Thienylboronic acid: Conformational search, molecular structure, NBO, NLO and FT-IR, FT-Raman, NMR and UV spectral analysis. Journal of Molecular Structure, 2014, 1076, 639-650.	3.6	10
31	FT-IR, FT-Raman, NMR, UV and quantum chemical studies on monomeric and dimeric conformations of 3,5-dimethyl-4-methoxybenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 352-362.	3.9	28
32	Spectroscopic (FT-IR, FT-Raman, and UVâ€“visible) and quantum chemical studies on molecular geometry, Frontier molecular orbitals, NBO, NLO and thermodynamic properties of 1-acetylindole. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 626-638.	3.9	17
33	FT-IR, FT-Raman and UV spectroscopic investigation, electronic properties, electric moments, and NBO analysis of anethole using quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 133, 165-177.	3.9	17
34	An experimental and theoretical investigation of Acenaphthene-5-boronic acid: Conformational study, NBO and NLO analysis, molecular structure and FT-IR, FT-Raman, NMR and UV spectra. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 753-766.	3.9	27
35	Molecular structure, electronic properties, NLO, NBO analysis and spectroscopic characterization of Gabapentin with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 109, 298-307.	3.9	38
36	Structural and spectroscopic characterization of a novel potential chemotherapeutic agent 3-(1-adamantyl)-1-{[4-(2-methoxyphenyl)piperazin-1-yl]methyl}-4-methyl-1H-1,2,4-triazole-5(4H)-thione by first principle calculations. Journal of Molecular Structure, 2012, 1022, 49-60.	3.6	37

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37	Monomeric and dimeric structures, electronic properties and vibrational spectra of azelaic acid by HF and B3LYP methods. Journal of Molecular Structure, 2012, 1022, 81-88.	3.6	8
38	The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMOâ€“LUMO analysis of monomeric and dimeric structures of 4-chloro-3,5-dinitrobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 93, 33-46.	3.9	106
39	Electronic structure, electric moments and vibrational analysis of 5-nitro-2-furaldehyde semicarbazone: A D.F.T. study. Computational and Theoretical Chemistry, 2011, 973, 20-27.	2.5	19
40	Raman, FT-IR spectroscopic analysis and first-order hyperpolarisability of 3-benzoyl-5-chlorouracil by first principles. Molecular Simulation, 2011, 37, 153-163.	2.0	123
41	Analysis of vibrational, structural, and electronic properties of rivastigmine by density functional theory. Journal of Applied Spectroscopy, 2010, 77, 468-478.	0.7	1
42	Molecular structure and vibrational study on 2,3-dihydro-1H-indene and its derivative 1H-indene-1,3(2H)-dione by density functional theory calculations. Computational and Theoretical Chemistry, 2010, 940, 82-86.	1.5	74
43	Electronic structure, non-linear properties and vibrational analysis of Acenaphthene and its carbonyl derivative Acenaphthenequinone by density functional theory. Computational and Theoretical Chemistry, 2010, 958, 33-40.	1.5	17
44	Vibrational analysis of deoxy-andrographolide using MM/QM methods. Spectroscopy, 2007, 21, 279-292.	0.8	1
45	Molecular structure and vibrational spectra of 2-formyl benzonitrile by density functional theory and ab initio Hartreeâ€“Fock calculations. Computational and Theoretical Chemistry, 2007, 822, 45-47.	1.5	21
46	FT-IR spectra and vibrational spectroscopy of Andrographolide. Spectroscopy, 2006, 20, 275-283.	0.8	11
47	Theoretical study of temperature induced transition and hyper stability of collagen mimics. Polymer, 2006, 47, 1674-1677.	3.8	6
48	Stereo-stability and temperature induced transitions of collagen mimics. Polymer, 2006, 47, 5360-5363.	3.8	0
49	Theoretical study of temperature induced phase transitions in poly(Î²-benzyl-l-aspartate) and it's copolymer. Polymer, 2005, 46, 7450-7455.	3.8	5
50	Pressure induced orderâ€“disorder transition in a diblock copolymer. Polymer, 2005, 46, 11876-11880.	3.8	3