

Leena Sinha

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8916100/publications.pdf>

Version: 2024-02-01

50
papers

983
citations

471509

17
h-index

454955

30
g-index

50
all docs

50
docs citations

50
times ranked

1028
citing authors

#	ARTICLE	IF	CITATIONS
1	Raman, FT-IR spectroscopic analysis and first-order hyperpolarisability of 3-benzoyl-5-chlorouracil by first principles. <i>Molecular Simulation</i> , 2011, 37, 153-163.	2.0	123
2	The spectroscopic (FT-Raman, FT-IR, UV and NMR), molecular electrostatic potential, polarizability and hyperpolarizability, NBO and HOMO-LUMO analysis of monomeric and dimeric structures of 4-chloro-3,5-dinitrobenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2012, 93, 33-46.	3.9	106
3	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. <i>Computational and Theoretical Chemistry</i> , 2010, 940, 82-86.	1.5	74
4	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 135, 283-295.	3.9	54
5	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. <i>Journal of Molecular Structure</i> , 2017, 1137, 725-741.	3.6	47
6	Virtual screening in drug-likeness and structure/activity relationship of pyridazine derivatives as Anti-Alzheimer drugs. <i>Journal of King Saud University - Science</i> , 2019, 31, 595-601.	3.5	41
7	Molecular structure, electronic properties, NLO, NBO analysis and spectroscopic characterization of Gabapentin with experimental (FT-IR and FT-Raman) techniques and quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 109, 298-307.	3.9	38
8	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. <i>Journal of Molecular Structure</i> , 2012, 1022, 49-60.	3.6	37
9	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. <i>Molecular Simulation</i> , 2019, 45, 1029-1043.	2.0	33
10	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. <i>European Journal of Medicinal Chemistry</i> , 2015, 92, 191-201.	5.5	30
11	FT-IR, FT-Raman, NMR, UV and quantum chemical studies on monomeric and dimeric conformations of 3,5-dimethyl-4-methoxybenzoic acid. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 123, 352-362.	3.9	28
12	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 753-766.	3.9	27
13	Molecular structure and vibrational spectra of 2-formyl benzonitrile by density functional theory and ab initio Hartree-Fock calculations. <i>Computational and Theoretical Chemistry</i> , 2007, 822, 45-47.	1.5	21
14	Structural, spectroscopic (FT-IR, FT-Raman and UV) studies, HOMO-LUMO, NBO, NLO analysis and reactivity descriptors of 2,3 Difluoroaniline and 2,4-Difluoroaniline. <i>Journal of Molecular Structure</i> , 2014, 1074, 457-466.	3.6	21
15	Electronic structure, electric moments and vibrational analysis of 5-nitro-2-furaldehyde semicarbazone: A D.F.T. study. <i>Computational and Theoretical Chemistry</i> , 2011, 973, 20-27.	2.5	19
16	Electronic structure, non-linear properties and vibrational analysis of Acenaphthene and its carbonyl derivative Acenaphthenequinone by density functional theory. <i>Computational and Theoretical Chemistry</i> , 2010, 958, 33-40.	1.5	17
17	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 124, 108-123.	3.9	17
18	Spectroscopic (FT-IR, FT-Raman, and UV-visible) and quantum chemical studies on molecular geometry, Frontier molecular orbitals, NBO, NLO and thermodynamic properties of 1-acetylindole. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 133, 626-638.	3.9	17

#	ARTICLE	IF	CITATIONS
19	FT-IR, FT-Raman and UV spectroscopic investigation, electronic properties, electric moments, and NBO analysis of anethole using quantum chemical calculations. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 133, 165-177.	3.9	17
20	DFT Study on the Electronic Properties, Spectroscopic Profile, and Biological Activity of 2-Amino-5-trifluoromethyl-1,3,4-thiadiazole with Anticancer Properties. <i>ACS Omega</i> , 2020, 5, 30073-30087.	3.5	17
21	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 140, 1-14.	3.9	15
22	Study on molecular structure, spectroscopic behavior, NBO, and NLO analysis of 3-methylbezothiazole-2-thione. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 146, 129-141.	3.9	15
23	Quantum-chemical (DFT, MP2) and spectroscopic studies (FT-IR and UV) of monomeric and dimeric structures of 2(3H)-Benzothiazolone. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 120, 126-136.	3.9	14
24	Syntheses, structural elucidation, thermal properties, theoretical quantum chemical studies (DFT) and biological studies of barbituricâ€“hydrazone complexes. <i>Journal of Saudi Chemical Society</i> , 2015, 19, 217-226.	5.2	14
25	FT-IR spectra and vibrational spectroscopy of Andrographolide. <i>Spectroscopy</i> , 2006, 20, 275-283.	0.8	11
26	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. <i>Journal of Molecular Structure</i> , 2014, 1076, 639-650.	3.6	10
27	Thermodynamic, spectroscopic and DFT studies of binary mixtures of poly(vinylpyrrolidone) (PVP) with ethanol, 1-propanol and 1-butanol. <i>Journal of Molecular Liquids</i> , 2020, 299, 112237.	4.9	10
28	Surface modification and characterization of h-BN-doped PVP thin film and its application as humidity sensor with theoretical DFT calculations. <i>Chemical Papers</i> , 2021, 75, 4055-4068.	2.2	9
29	Monomeric and dimeric structures, electronic properties and vibrational spectra of azelaic acid by HF and B3LYP methods. <i>Journal of Molecular Structure</i> , 2012, 1022, 81-88.	3.6	8
30	Exploring QSARs of some benzenesulfonamides incorporating cyanoacrylamide moieties as a carbonic anhydrase inhibitors (specifically against tumor-associated isoforms IX and XII). <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2015, 30, 519-523.	5.2	8
31	Spectroscopic and electronic structure calculation of a potential antibacterial agent incorporating pyrido-dipyrimidine-dione moiety using first principles. <i>Journal of Molecular Structure</i> , 2016, 1110, 128-137.	3.6	8
32	A Combined theoretical and experimental study of conformational and spectroscopic profile of 2-acetamido-5-aminopyridine. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2015, 143, 147-157.	3.9	7
33	Structure Activity Relationship and Quantitative Structure-Activity Relationships Modeling of Antitrypanosomal Activities of Alkyldiamine Cryptolepine Derivatives. <i>Journal of Computational and Theoretical Nanoscience</i> , 2015, 12, 2421-2427.	0.4	7
34	Prediction of molecular properties and spectroscopic profile of Riluzole with different functionals (B3LYP, M06-2X, MPWLYP): A combined theoretical and experimental study. <i>Journal of Molecular Structure</i> , 2016, 1106, 265-276.	3.6	7
35	Theoretical study of temperature induced transition and hyper stability of collagen mimics. <i>Polymer</i> , 2006, 47, 1674-1677.	3.8	6
36	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. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2014, 132, 568-581.	3.9	6

#	ARTICLE	IF	CITATIONS
37	Theoretical study of temperature induced phase transitions in poly(^l -benzyl-l-aspartate) and it's copolymer. <i>Polymer</i> , 2005, 46, 7450-7455.	3.8	5
38	Spectral investigation and theoretical study of zwitterionic and neutral forms of quinolinic acid. <i>Journal of Molecular Structure</i> , 2015, 1095, 100-111.	3.6	5
39	Spectroscopic and electronic structure calculation of a potential chemotherapeutic agent 5-propyl-6-(p-tolylsulfanyl)pyrimidine-2,4(1H,3H)-dione using first principles. <i>Journal of Molecular Structure</i> , 2015, 1100, 225-236.	3.6	5
40	Conformational search, spectral analysis and electronic properties of 5-(4-Pyridinyl)-1,3,4-thiadiazol-2-amine. <i>Journal of Molecular Structure</i> , 2016, 1108, 112-125.	3.6	5
41	Investigations on Molecular Structure, Electronic Properties, NLO Properties and Comparison of Drug-Likeness of Triazolothiadiazole Derivatives by Quantum Methods and QSAR Analysis. <i>Reviews in Theoretical Science</i> , 2016, 4, 85-96.	0.5	5
42	Thermoacoustic and DFT Analysis of N,N-Dimethylacetamide (DMA) with 1-Propanol and Methanol at 293.15, 303.15, and 313.15K. <i>Brazilian Journal of Physics</i> , 2021, 51, 515-526.	1.4	4
43	Pressure induced order-disorder transition in a diblock copolymer. <i>Polymer</i> , 2005, 46, 11876-11880.	3.8	3
44	Conformational and spectroscopic behaviors of 2,4-xylyl isothiocyanate. <i>Journal of Molecular Structure</i> , 2015, 1087, 113-120.	3.6	3
45	First principle study of a potential bioactive molecule with tetrahydroisoquinoline, carbothiomide and adamantane scaffolds. <i>Journal of Molecular Structure</i> , 2017, 1143, 204-216.	3.6	3
46	Spectroscopic, electronic structure, molecular docking, and molecular dynamics simulation study of 7-Trifluoromethyl-1H-indole-2-carboxylic acid as an aromatase inhibitor. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2022, 280, 121530.	3.9	3
47	Vibrational analysis of deoxy-andrographolide using MM/QM methods. <i>Spectroscopy</i> , 2007, 21, 279-292.	0.8	1
48	Analysis of vibrational, structural, and electronic properties of rivastigmine by density functional theory. <i>Journal of Applied Spectroscopy</i> , 2010, 77, 468-478.	0.7	1
49	Study of molecular association in binary mixtures of poly(vinyl pyrrolidone) (PVP) with ethanol, 1-propanol and 1-butanol through thermo-acoustical, FT-IR, UV-Vis spectroscopy and DFT studies. <i>European Physical Journal D</i> , 2021, 75, 1.	1.3	1
50	Stereo-stability and temperature induced transitions of collagen mimics. <i>Polymer</i> , 2006, 47, 5360-5363.	3.8	0