Meganathan

List of Publications by Year
in descending order

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37 papers	917 citations	471509 17 h-index	454955 30 g-index
37 all docs	37 docs citations	37 times ranked	933 citing authors

#	Article	IF	Citations
1	FT-IR, FT-Raman spectra and ab initio HF and DFT calculations of 4-N,Nâ€²-dimethylamino pyridine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 898-906.	3.9	144
2	Molecular structure and vibrational spectra of 3-chloro-4-fluoro benzonitrile by ab initio HF and density functional method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 71, 1134-1139.	3.9	80
3	Molecular structure, spectroscopic (FTIR, FTIR gas phase, FTâ€Raman) firstâ€order hyperpolarizability and HOMOâ€“LUMO analysis of 4â€methoxyâ€2â€methyl benzoic acid. Journal of Raman Spectroscopy, 2010, 41, 1369-1378.	2.5	68
4	FT-IR, FT-Raman spectra and ab initio HF, DFT vibrational analysis of 2,3-difluoro phenol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 561-566.	3.9	61
5	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 3-aminobenzotrifluoride. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 214-224.	3.9	47
6	FT-IR, FT-Raman spectra and ab initio HF, DFT vibrational analysis of p-chlorobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 871-879.	3.9	47
7	Molecular structure and vibrational spectra of indole and 5-aminoindole by density functional theory and ab initio Hartreeâ€“Fock calculations. Computational and Theoretical Chemistry, 2008, 850, 84-93.	1.5	45
8	Molecular structure and vibrational spectra of 2-amino-5-methyl pyridine and 2-amino-6-methyl pyridine by density functional methods. Journal of Molecular Structure, 2008, 891, 284-291.	3.6	45
9	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 2-amino-4,6-dimethoxypyrimidine. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 65, 1186-1196.	3.9	44
10	Vibrational spectra and quantum chemical calculations of 3,4-diaminobenzoic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 376-383.	3.9	33
11	FT-IR, FT-Raman spectra and ab initio DFT vibrational analysis of p-bromophenoxyacetic acid. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 66, 773-780.	3.9	31
12	Vibrational spectra and assignments of 3-aminobenzyl alcohol by ab initio Hartreeâ€“Fock and density functional method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 69, 198-204.	3.9	26
13	Pharmacophore modeling, virtual screening, molecular docking studies and density functional theory approaches to identify novel ketohexokinase (KHK) inhibitors. BioSystems, 2015, 138, 39-52.	2.0	25
14	Identification of Important Chemical Features of 11Î²-Hydroxysteroid Dehydrogenase Type1 Inhibitors: Application of Ligand Based Virtual Screening and Density Functional Theory. International Journal of Molecular Sciences, 2012, 13, 5138-5162.	4.1	24
15	Vibrational spectra and assignments of 2-amino-5-iodopyridine by ab initio Hartreeâ€“Fock and density functional methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 67, 830-836.	3.9	20
16	FT-IR, FT-Raman spectra and quantum chemical calculations of 3,4-dimethoxyaniline. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 50-59.	3.9	18
17	Molecular structure, vibrational spectra and HOMO, LUMO analysis of 4-piperidone by density functional theory andab initioHartreeâ€“Fock calculations. Molecular Simulation, 2009, 35, 705-713.	2.0	18
18	FT-IR, FT-Raman spectra and quantum chemical calculations of some chloro substituted phenoxy acetic acids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2008, 70, 430-438.	3.9	16

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19	Molecular modeling study for conformational changes of Sirtuin 2 due to substrate and inhibitor binding. Journal of Biomolecular Structure and Dynamics, 2012, 30, 235-254.	3.5	16
20	Vibrational spectroscopy investigation using ab initio and density functional theory analysis on the structure of 5-amino-o-cresol. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2007, 68, 619-625.	3.9	15
21	Rhizopus stolonifer mediated biosynthesis of biocompatible cadmium chalcogenide quantum dots. Enzyme and Microbial Technology, 2016, 95, 225-229.	3.2	13
22	Structural, vibrational (FT-IR and FT-Raman) and UVâ€“Vis spectral analysis of 1-phenyl-3-(1,2,3-thiadiazol-5-yl)urea by DFT method. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2012, 95, 331-340.	3.9	12
23	Vibrational and conformational analysis on-N1-N2-bis((pyridine-4-yl)methylene) benzene-1,2-diamine. Journal of Molecular Structure, 2013, 1042, 37-44.	3.6	11
24	Combined ligand based pharmacophore modeling, virtual screening methods to identify critical chemical features of novel potential inhibitors for phosphodiesterase-5. Journal of the Taiwan Institute of Chemical Engineers, 2011, 42, 709-718.	5.3	10
25	Investigation on the isoform selectivity of novel kinesin-like protein 1 (KIF11) inhibitor using chemical feature based pharmacophore, molecular docking, and quantum mechanical studies. Computational Biology and Chemistry, 2016, 61, 47-61.	2.3	8
26	Insight Mechanism of the Selective Lanosterol Synthase Inhibitor: Molecular Modeling, Docking and Density Functional Theory Approaches. Current Computer-Aided Drug Design, 2017, 13, 275-293.	1.2	8
27	Molecular Dynamics Simulation Study for Ionic Strength Dependence of RNA-host factor Interaction in Staphylococcus aureus Hfq. Bulletin of the Korean Chemical Society, 2010, 31, 1519-1526.	1.9	8
28	Synthesis and evaluation of the antagonistic activity of 3-acetyl-2H-benzo[g]chromen-2-one against mutant Y537S estrogen receptor alpha via E-Pharmacophore modeling, molecular docking, molecular dynamics, and in-vitro cytotoxicity studies. Journal of Molecular Structure, 2021, 1224, 129289.	3.6	6
29	Combined chemical feature-based assessment and Bayesian model studies to identify potential inhibitors for Factor Xa. Medicinal Chemistry Research, 2012, 21, 4083-4099.	2.4	4
30	Pharmacophore Design, Virtual Screening, Molecular Docking and Optimization Approaches to Discover Potent Thrombin Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2013, 16, 702-720.	1.1	4
31	Discovery of potent inhibitors for interleukin-2-inducible T-cell kinase: structure-based virtual screening and molecular dynamics simulation approaches. Journal of Molecular Modeling, 2013, 19, 715-726.	1.8	3
32	Pharmacophore Design for Anti-inflammatory Agent Targeting Interleukin-2 Inducible Tyrosine Kinase (Itk). Bulletin of the Korean Chemical Society, 2010, 31, 3333-3340.	1.9	3
33	Ligand Based Pharmacophore Identification and Molecular Docking Studies for Grb2 Inhibitors. Bulletin of the Korean Chemical Society, 2012, 33, 1707-1714.	1.9	3
34	Atom Based 3D-QSAR, Molecular Docking and Density Functional Theory Approaches to Identify Novel JNK-1 Inhibitor. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 771-797.	1.1	1
35	Molecular structure and vibrational spectra of 4-nitrobenzylchloride byab initioHartreeâ€“Fock and density functional methods. Molecular Simulation, 2008, 34, 619-630.	2.0	0
36	Pharmacophore based virtual screening, molecular docking and density functional theory approaches to discover the potent beta-amyloid precursor protein (B-APP) inhibitor. AIP Conference Proceedings, 2019, , .	0.4	0

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37	3D-QSAR modeling, molecular docking and quantum mechanical approaches to identify pleckstrin homology domain of new AKT1 inhibitors. AIP Conference Proceedings, 2019, , .	0.4	0