M Prasath

List of Publications by Year
in descending order

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16	214	933447 10	1058476 14
papers	citations	h-index	g-index

16	16	16	111
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Donor functionalized perylene and different Ï€-spacer based sensitizers for dye-sensitized solar cell applications â€" a theoretical approach. Journal of Molecular Modeling, 2022, 28, 102.	1.8	6
2	Spectroscopic, quantum chemical, ADMET and molecular docking studies of echinatin: a prospective tuberculosis drug. Research on Chemical Intermediates, 2022, 48, 2363-2390.	2.7	5
3	Quantum chemical calculations, spectroscopic studies and molecular docking investigations of the anti-cancer drug quercitrin with B-RAF inhibitor. Heliyon, 2022, 8, e09539.	3.2	10
4	Spectroscopic (FT-IR, FT-Raman) investigations, quantum chemical calculations, ADMET and molecular docking studies of phloretin with B-RAF inhibitor. Chemical Papers, 2021, 75, 3771-3785.	2.2	10
5	Exploring the molecular structure, vibrational spectroscopic, quantum chemical calculation and molecular docking studies of curcumin: A potential PI3K/AKT uptake inhibitor. Heliyon, 2021, 7, e06646.	3.2	13
6	Exploring the screening of perylene based organic sensitizers with different lengths and functional groups of acceptors via computational spectroscopic analysis. Chemical Data Collections, 2021, 34, 100729.	2.3	5
7	Vibrational spectra, Hirshfeld surface analysis, molecular docking studies of (RS)-N,N-bis(2-chloroethyl)-1,3,2-oxazaphosphinan-2-amine 2-oxide by DFT approach. Heliyon, 2020, 6, e04641.	3.2	16
8	Probing the vibrational spectroscopic properties and binding mechanism of anti-influenza agent Liquiritin using experimental and computational studies. Research on Chemical Intermediates, 2020, 46, 4475-4507.	2.7	18
9	Vibrational Analysis (FT-IR and FT-Raman Spectra) and Molecular Docking Evaluation of MPTB in GABA Receptor. Journal of Cluster Science, 2019, 30, 1025-1035.	3.3	15
10	Invivo, molecular docking, spectroscopy studies of (S)-2,3-Dihydro-5,7-dihydroxy-2(3-hydroxy-4-methoxyphenyl)-4H-1-benzopyran-4-one: A potential uptake PI3/AKT inhibitor. Biocatalysis and Agricultural Biotechnology, 2019, 18, 101086.	3.1	17
11	Spectroscopic (FT-IR, FT-Raman, UVâ€"Vis), quantum chemical calculation and molecular docking evaluation of liquiritigenin: an influenza A (H1N1) neuraminidase inhibitor. Research on Chemical Intermediates, 2019, 45, 2135-2166.	2.7	21
12	Spectroscopic investigations (FT-IR & FT-Raman) and molecular docking analysis of 292-300.	3.6	14
13	FT-IR, FT-Raman spectra and ab initio HF and DFT calculations of 7-chloro-5-(2-chlorophenyl)-3-hydroxy-2,3-dihydro-1H-1,4-benzodiazepin-2-one. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 120, 185-194.	3.9	25
14	Quantum chemical studies, vibrational analysis, molecular structure, first order hyper polarizability, NBO and HOMOâ€"LUMO analysis of 3-hydroxybenzaldehyde and its cation. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 115, 789-799.	3.9	17
15	Vibrational spectroscopy investigation using ab initio and DFT vibrational analysis of 7-chloro-2-methylamino-5-phenyl-3H-1,4-benzodiazepine-4-oxide. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 113, 224-235.	3.9	19
16	Vibrational Assignments, First-Order Hyperpolarizability and Molecular Structure of 5-(2-Chlorphenyl)-7-nitro-2,3-dihydro-1,4-benzodiazepine-2-one by Hartree-Fock and Density Functional Theory Calculations. Asian Journal of Chemistry, 2013, 25, 6771-6776.	0.3	3