Palanisamy Deepa

List of Publications by Year
in descending order

30	366	759233 12	794594 19
papers	citations	h-index	g-index

30	30	30	323
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Rising trend on the halogen and non-halogen derivatives (Br, Cl, CF₃, F, CH₃) Tj ETQq1 1 0.784314 rgBT /O Biomolecular Structure and Dynamics, 2022, 40, 449-467.	3.5	1
2	Understanding the impact of anticancer halogenated inhibitors and various functional groups (Xâ€‰=â€‰Cl,) Tj ETQq0 0 0 rgBT /Over Biomolecular Structure and Dynamics, 2022, 40, 5036-5052.	3.5	1
3	A quantum chemical perspective on the potency of electron donors and acceptors in pnicogen bonds (AS...N, P...N, N...N). Journal of Molecular Modeling, 2020, 26, 11.	1.8	5
4	Understanding the potency of malarial ligand (D44) in plasmodium FKBP35 and modelled halogen atom (Br, Cl, F) functional groups. Journal of Molecular Graphics and Modelling, 2020, 97, 107553.	2.4	5
5	Does the stability of the stacking motif surpass the planar motif in 2-amino-4-nitrophenol? â€" a CCSD(T) analysis. Journal of Molecular Modeling, 2019, 25, 6.	1.8	1
6	An overview about the impact of hinge region towards the anticancer binding affinity of the Ck2 ligands: a quantum chemical analysis. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3859-3876.	3.5	3
7	Does the presence of water clusters induce the binding affinity of CK2 halogen ligands?: A quantum chemical perspective study. International Journal of Quantum Chemistry, 2018, 118, e25644.	2.0	6
8	Synthesis and Experimental Studies on Supramolecular Synthons of Aminoguanidinium Carboxylates: A Case Study of Ï€â€HoleBonded Carbon Bonding via Theoretical Approaches. ChemistrySelect, 2018, 3, 10032-10048.	1.5	1
9	Hybrid DFT study on non-covalent interactions and their influence on pKa's of magnesium-carboxylate complexes. Journal of Molecular Graphics and Modelling, 2018, 85, 13-24.	2.4	5
10	An Overview of the Factors Influencing CK2 Ligands and the Impact of Crystal Waters: A Theoretical Study. Crystal Growth and Design, 2017, 17, 1299-1315.	3.0	8
11	Understanding the potency of fatty acids with the amino acid side chains of bovine Î² lactoglobulinâ€"A quantum chemical approach. Journal of Molecular Graphics and Modelling, 2017, 74, 105-116.	2.4	7
12	Understanding the nature of Metal Oxalato Complexes with Purine Nucleobase- A Quantum Chemical approach. International Journal of Molecular and Theoretical Physics, 2017, 1, 1-10.	0.3	0
13	Topological analysis of metalâ€"ligand and hydrogen bonds in transition metal hybrid structures â€" A computational study. Polyhedron, 2016, 115, 193-203.	2.2	4
14	Studies on the Ïƒâ€"hole bonds (halogen, chalcogen, pnicogen and carbon bonds) based on the orientation of crystal structure. Molecular Physics, 2016, 114, 3629-3642.	1.7	20
15	Does the occurrence of resonance (by the delocalization of radical/cationic/anionic charges) induce the existence of intramolecular halogenâ€"halogen contacts?. RSC Advances, 2016, 6, 66870-66878.	3.6	6
16	Do resonance-assisted intramolecular halogen bonds exist without a charge transfer and a Ïƒ-hole?. Physical Chemistry Chemical Physics, 2015, 17, 27496-27508.	2.8	26
17	Characteristics of a Ïƒ-Hole and the Nature of a Halogen Bond. Topics in Current Chemistry, 2014, 359, 1-25.	4.0	19
18	On the origin of the substantial stabilisation of the electron-donor 1,3-dithiole-2-thione-4-carboxyclic acidâ‹¯I₂and DABCOâ‹¯I₂complexes. Physical Chemistry Chemical Physics, 2014, 16, 6679-6686.	2.8	31

#	Article	IF	Citations
19	On the nature of non-covalent interactions in isomers of 2,5-dichloro-1,4-benzoquinone dimers â€“ ground- and excited-state properties. Physical Chemistry Chemical Physics, 2014, 16, 19928-19940.	2.8	16
20	Halogen bonds in crystal TTF derivatives: an ab initio quantum mechanical study. Physical Chemistry Chemical Physics, 2014, 16, 2038-2047.	2.8	46
21	The nature of hydrogen bonding inR²₂(8) crystal motifs â€“ a computational exploration. Molecular Physics, 2014, 112, 3195-3205.	1.7	14
22	A theoretical perspective of the nature of hydrogen-bond types â€“ the atoms in molecules approach. Molecular Physics, 2014, 112, 1609-1623.	1.7	15
23	Why Is the L-Shaped Structure of X₂Â·Â·Â·X₂ (X = F, Cl, Br, I) Complexes More Stable Than Other Structures?. Journal of Physical Chemistry A, 2014, 118, 3846-3855.	2.5	21
24	Structural properties and the effect of platinum drugs with DNA base pairs. Structural Chemistry, 2013, 24, 583-595.	2.0	13
25	Theoretical investigation of interaction between psoralen and altretamine with stacked DNA base pairs. Materials Science and Engineering C, 2012, 32, 423-431.	7.3	25
26	Hydrogen-bonding studies of amino acid side-chains with DNA base pairs. Molecular Physics, 2011, 109, 1995-2008.	1.7	10
27	Structural properties and the effect of 2,6â€diaminoanthraquinone on Gâ€tetrad, nonâ€Gâ€tetrads, and mixed tetradsâ€”A density functional theory study. International Journal of Quantum Chemistry, 2011, 111, 3239-3250.	2.0	8
28	First and second coordination spheres in 8-azaxanthinato salts of divalent metal aquacomplexes â€“ Ab initio and DFT study. Polyhedron, 2011, 30, 1431-1445.	2.2	8
29	Interactions of anticancer drugs with usual and mismatch base pairs â€” Density functional theory studies. Biophysical Chemistry, 2008, 136, 50-58.	2.8	26
30	Studies on Tautomeric Forms of Guanine-Cytosine Base Pairs of Nucleic Acids and Their Interactions with Water Molecules. Journal of Biomolecular Structure and Dynamics, 2008, 25, 733-746.	3.5	15