Zahra Aliakbar Tehrani

List of Publications by Year
in descending order

34 papers	503 citations	687363 13 h-index	713466 21 g-index
34 all docs	34 docs citations	34 times ranked	828 citing authors

#	Article	IF	Citations
1	Molecular dynamics simulations provide structural insight into binding of cyclic dinucleotides to human STING protein. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10250-10264.	3.5	5
2	Conformational energies and equilibria of cyclic dinucleotidesin vacuoand in solution: computational chemistryvs.NMR experiments. Physical Chemistry Chemical Physics, 2021, 23, 7280-7294.	2.8	5
3	Proteinâ€“Ligand Interactions in the STING Binding Site Probed by Rationally Designed Single-Point Mutations: Experiment and Theory. Biochemistry, 2021, 60, 607-620.	2.5	15
4	Ligand Strain and Its Conformational Complexity Is a Major Factor in the Binding of Cyclic Dinucleotides to STING Protein. Angewandte Chemie - International Edition, 2021, 60, 10172-10178.	13.8	22
5	Ligand Strain and Its Conformational Complexity Is a Major Factor in the Binding of Cyclic Dinucleotides to STING Protein. Angewandte Chemie, 2021, 133, 10260-10266.	2.0	3
6	Enzymatic Preparation of 2â€²â€“5â€²,3â€²â€“5â€²-Cyclic Dinucleotides, Their Binding Properties to Stimulator of Interferon Genes Adaptor Protein, and Structure/Activity Correlations. Journal of Medicinal Chemistry, 2019, 62, 10676-10690.	6.4	45
7	Halides with Fifteen Aliphatic Câ€“HÂ·Â·Â·Anion Interaction Sites. Scientific Reports, 2016, 6, 30123.	3.3	7
8	Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimerâ€™s disease. Nature Communications, 2016, 7, 13115.	12.8	80
9	Functional molecules and materials by Ï€â€“interaction based quantum theoretical design. International Journal of Quantum Chemistry, 2016, 116, 622-633.	2.0	29
10	Intriguing Electrostatic Potential of CO: Negative Bond-ends and Positive Bond-cylindrical-surface. Scientific Reports, 2015, 5, 16307.	3.3	29
11	Interactions of small gold clusters, Aun (n=1â€“3), with graphyne: Theoretical investigation. Journal of Molecular Graphics and Modelling, 2014, 54, 80-89.	2.4	21
12	Watsonâ€“Crick versus imidazopyridopyrimidine base pairs: theoretical study on differences in stability and hydrogen bonding strength. Structural Chemistry, 2014, 25, 1271-1280.	2.0	3
13	Glucose interaction with Au, Ag, and Cu clusters: Theoretical investigation. International Journal of Quantum Chemistry, 2013, 113, 1062-1070.	2.0	21
14	Do coinage metal anions interact with substituted benzene derivatives?. Journal of Molecular Modeling, 2013, 19, 4763-4772.	1.8	8
15	Theoretical Investigation on Antioxidant Activity of Bromophenols from the Marine Red Alga Rhodomela confervoides: H-Atom vs Electron Transfer Mechanism. Journal of Agricultural and Food Chemistry, 2013, 61, 1534-1541.	5.2	32
16	Conformational aspects of glutathione tripeptide: electron density topological & natural bond orbital analyses. Structural Chemistry, 2013, 24, 147-158.	2.0	5
17	Computational investigation of thermochemical properties of non-natural C-nucloebases: different hydrogen-bonding preferences for non-natural Watsonâ€“Crick base pairs. Structural Chemistry, 2013, 24, 1015-1025.	2.0	5
18	Comparison of gas phase intrinsic properties of cytosine and thymine nucleobases with their O-alkyl adducts: different hydrogen bonding preferences for thymine versus O-alkyl thymine. Journal of Molecular Modeling, 2013, 19, 2993-3005.	1.8	4

#	Article	IF	Citations
19	Interactions of coinage metal clusters with histidine and their effects on histidine acidity; theoretical investigation. Organic and Biomolecular Chemistry, 2012, 10, 9373.	2.8	9
20	Influence of metal complexation on acidity of cytosine nucleosides: Part I, Li+, Na+ and K+ cation. Scientia Iranica, 2012, 19, 535-545.	0.4	2
21	Interactions of Glutathione Tripeptide with Gold Cluster: Influence of Intramolecular Hydrogen Bond on Complexation Behavior. Journal of Physical Chemistry A, 2012, 116, 4338-4347.	2.5	42
22	Can anion interaction accelerate transformation of cytosine tautomers? Detailed view form QTAIM analysis. Structural Chemistry, 2012, 23, 1843-1855.	2.0	2
23	Experimental and Computational Bridgehead Câ€“H Bond Dissociation Enthalpies. Journal of Organic Chemistry, 2012, 77, 1909-1914.	3.2	9
24	EFFECT OF CATION RADICAL FORMATION ON REACTIVITY AND ACIDITY ENHANCEMENT OF CYTOSINE NUCLEOBASE: NATURAL BOND ORBITAL AND ATOM IN MOLECULE ANALYSIS. Journal of Theoretical and Computational Chemistry, 2012, 11, 313-327.	1.8	11
25	What roles do boron substitutions play in structural, tautomeric, base pairing and electronic properties of uracil? NBO & AIM analysis. Journal of Physical Organic Chemistry, 2012, 25, 787-796.	1.9	4
26	How hydrogenâ€bonded MnO₄^{â€} can influence oxidation of olefins in both gas phase and solution?. Journal of Physical Organic Chemistry, 2012, 25, 1198-1209.	1.9	4
27	Thermochemical properties of some vinyl chloride-induced DNA lesions: detailed view from NBO & AIM analysis. Structural Chemistry, 2012, 23, 1987-2001.	2.0	3
28	Structural behavior of sugar radicals formed by proton transfer reaction of deoxycytidine cation radical: detailed view from NBO analysis. Structural Chemistry, 2012, 23, 1185-1192.	2.0	2
29	Structures, stabilities & conformational behaviors of hydrogen-atom abstractions of cytosine nucleosides: AIM & NBO analysis. Computational and Theoretical Chemistry, 2011, 971, 19-29.	2.5	7
30	DFT STUDY ON CONFORMATIONAL BEHAVIOR OF HYDROGEN ION ABSTRACTIONS OF CYTOSINE NUCLEOSIDES: AIM AND NBO ANALYSIS. Journal of Theoretical and Computational Chemistry, 2011, 10, 803-817.	1.8	3
31	Conformational behavior and potential energy profile of gaseous histidine. Computational and Theoretical Chemistry, 2010, 960, 73-85.	1.5	20
32	Interaction of Mg2+, Ca2+, Zn2+ and Cu+ with cytosine nucleosides: Influence of metal on sugar puckering and stability of N-Glycosidic bond, a DFT study. Computational and Theoretical Chemistry, 2009, 913, 117-125.	1.5	22
33	Anion interactions of cytosine nucleobase and its nucleosides: Detailed view from DFT study. Computational and Theoretical Chemistry, 2009, 913, 277-283.	1.5	7
34	DFT study of the interaction of cytidine and 2â€²-deoxycytidine with Li+, Na+, and K+: effects of metal cationization on sugar puckering and stability of the N-glycosidic bond. Carbohydrate Research, 2009, 344, 771-778.	2.3	17