

Zahra Aliakbar Tehrani

List of Publications by Year in descending order

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34
papers

503
citations

687363

13
h-index

713466

21
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34
all docs

34
docs citations

34
times ranked

828
citing authors

#	ARTICLE	IF	CITATIONS
1	Structure-mechanism-based engineering of chemical regulators targeting distinct pathological factors in Alzheimer's disease. <i>Nature Communications</i> , 2016, 7, 13115.	12.8	80
2	Enzymatic Preparation of 2',3'-Cyclic Dinucleotides, Their Binding Properties to Stimulator of Interferon Genes Adaptor Protein, and Structure/Activity Correlations. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 10676-10690.	6.4	45
3	Interactions of Glutathione Tripeptide with Gold Cluster: Influence of Intramolecular Hydrogen Bond on Complexation Behavior. <i>Journal of Physical Chemistry A</i> , 2012, 116, 4338-4347.	2.5	42
4	Theoretical Investigation on Antioxidant Activity of Bromophenols from the Marine Red Alga <i>Rhodomela confervoides</i> : H-Atom vs Electron Transfer Mechanism. <i>Journal of Agricultural and Food Chemistry</i> , 2013, 61, 1534-1541.	5.2	32
5	Intriguing Electrostatic Potential of CO: Negative Bond-ends and Positive Bond-cylindrical-surface. <i>Scientific Reports</i> , 2015, 5, 16307.	3.3	29
6	Functional molecules and materials by π -interaction based quantum theoretical design. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 622-633.	2.0	29
7	Interaction of Mg ²⁺ , Ca ²⁺ , Zn ²⁺ and Cu ⁺ with cytosine nucleosides: Influence of metal on sugar puckering and stability of N-Glycosidic bond, a DFT study. <i>Computational and Theoretical Chemistry</i> , 2009, 913, 117-125.	1.5	22
8	Ligand Strain and Its Conformational Complexity Is a Major Factor in the Binding of Cyclic Dinucleotides to STING Protein. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 10172-10178.	13.8	22
9	Glucose interaction with Au, Ag, and Cu clusters: Theoretical investigation. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1062-1070.	2.0	21
10	Interactions of small gold clusters, Au _n (n=1-3), with graphyne: Theoretical investigation. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 54, 80-89.	2.4	21
11	Conformational behavior and potential energy profile of gaseous histidine. <i>Computational and Theoretical Chemistry</i> , 2010, 960, 73-85.	1.5	20
12	DFT study of the interaction of cytidine and 2'-deoxycytidine with Li ⁺ , Na ⁺ , and K ⁺ : effects of metal cationization on sugar puckering and stability of the N-glycosidic bond. <i>Carbohydrate Research</i> , 2009, 344, 771-778.	2.3	17
13	Protein-Ligand Interactions in the STING Binding Site Probed by Rationally Designed Single-Point Mutations: Experiment and Theory. <i>Biochemistry</i> , 2021, 60, 607-620.	2.5	15
14	EFFECT OF CATION RADICAL FORMATION ON REACTIVITY AND ACIDITY ENHANCEMENT OF CYTOSINE NUCLEOBASE: NATURAL BOND ORBITAL AND ATOM IN MOLECULE ANALYSIS. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 313-327.	1.8	11
15	Interactions of coinage metal clusters with histidine and their effects on histidine acidity; theoretical investigation. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 9373.	2.8	9
16	Experimental and Computational Bridgehead C-H Bond Dissociation Enthalpies. <i>Journal of Organic Chemistry</i> , 2012, 77, 1909-1914.	3.2	9
17	Do coinage metal anions interact with substituted benzene derivatives?. <i>Journal of Molecular Modeling</i> , 2013, 19, 4763-4772.	1.8	8
18	Anion interactions of cytosine nucleobase and its nucleosides: Detailed view from DFT study. <i>Computational and Theoretical Chemistry</i> , 2009, 913, 277-283.	1.5	7

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19	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
20	Halides with Fifteen Aliphatic C-H...Anion Interaction Sites. Scientific Reports, 2016, 6, 30123.	3.3	7
21	Conformational aspects of glutathione tripeptide: electron density topological & natural bond orbital analyses. Structural Chemistry, 2013, 24, 147-158.	2.0	5
22	Computational investigation of thermochemical properties of non-natural C-nucleobases: different hydrogen-bonding preferences for non-natural Watson-Crick base pairs. Structural Chemistry, 2013, 24, 1015-1025.	2.0	5
23	Conformational energies and equilibria of cyclic dinucleotides in vacuo and in solution: computational chemistry vs. NMR experiments. Physical Chemistry Chemical Physics, 2021, 23, 7280-7294.	2.8	5
24	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
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 hydrogen-bonded MnO ₄ ⁻ can influence oxidation of olefins in both gas phase and solution?. Journal of Physical Organic Chemistry, 2012, 25, 1198-1209.	1.9	4
27	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
28	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
29	Thermochemical properties of some vinyl chloride-induced DNA lesions: detailed view from NBO & AIM analysis. Structural Chemistry, 2012, 23, 1987-2001.	2.0	3
30	Watson-Crick versus imidazopyridopyrimidine base pairs: theoretical study on differences in stability and hydrogen bonding strength. Structural Chemistry, 2014, 25, 1271-1280.	2.0	3
31	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
32	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
33	Can anion interaction accelerate transformation of cytosine tautomers? Detailed view from QTAIM analysis. Structural Chemistry, 2012, 23, 1843-1855.	2.0	2
34	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