David Reha

List of Publications by Year
in descending order

35 papers	1,079 citations	471061 17 h-index	395343 33 g-index
36 all docs	36 docs citations	36 times ranked	1637 citing authors

#	Article	IF	Citations
1	Metallic Effects on p-Hydroxyphenyl Porphyrin Thin-Film-Based Planar Optical Waveguide Gas Sensor: Experimental and Computational Studies. Nanomaterials, 2022, 12, 944.	1.9	6
2	Interactions between a dsDNA Oligonucleotide and Imidazolium Chloride Ionic Liquids: Effect of Alkyl Chain Length, Part I. Molecules, 2022, 27, 116.	1.7	1
3	Surface Interaction of Ionic Liquids: Stabilization of Polyethylene Terephthalate-Degrading Enzymes in Solution. Molecules, 2022, 27, 119.	1.7	2
4	Substituent Effect on Porphyrin Film-Gas Interaction by Optical Waveguide: Spectrum Analysis and Molecular Dynamic Simulation. Materials, 2020, 13, 5613.	1.3	5
5	Conserved Dynamic Mechanism of Allosteric Response to L-arg in Divergent Bacterial Arginine Repressors. Molecules, 2020, 25, 2247.	1.7	3
6	Interstrand Charge Transport within Metallo-DNA: the Effect Due to Hg(II)- and Ag(I)-Mediated Base Pairs. Journal of Physical Chemistry C, 2020, 124, 7477-7486.	1.5	2
7	The study of conformational changes in photosystem II during a charge separation. Journal of Molecular Modeling, 2020, 26, 75.	0.8	9
8	From the vapor-liquid equilibrium to the supercritical condition. Molecular dynamics modeling of 1,3-butadiene. Journal of Molecular Liquids, 2020, 315, 113702.	2.3	4
9	Experimental and theoretical investigation of solvatochromic properties and ion solvation structure in DESs of reline, glyceline, ethaline and their mixtures with PEG 400. Journal of Molecular Liquids, 2019, 284, 59-67.	2.3	36
10	Aggregation and metal-complexation behaviour of THPP porphyrin in ethanol/water solutions as function of pH. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 193, 235-248.	2.0	29
11	A residue of motif III positions the helicase domains of motor subunit HsdR in restriction-modification enzyme EcoR124I. Journal of Molecular Modeling, 2018, 24, 176.	0.8	4
12	The mechanism of the glycosylase reaction with hOGG1 base-excision repair enzyme: concerted effect of Lys249 and Asp268 during excision of 8-oxoguanine. Nucleic Acids Research, 2017, 45, 5231-5242.	6.5	19
13	Theoretical and experimental study of the antifreeze protein AFP752, trehalose and dimethyl sulfoxide cryoprotection mechanism: correlation with cryopreserved cell viability. RSC Advances, 2017, 7, 352-360.	1.7	50
14	Transmembrane helix connectivity in Orai1 controls two gates for calcium-dependent transcription. Science Signaling, 2017, 10, .	1.6	68
15	The helical domain of the EcoR124I motor subunit participates in ATPase activity and dsDNA translocation. PeerJ, 2017, 5, e2887.	0.9	2
16	Influence of ligand binding on structure and thermostability of human Î±₁-acid glycoprotein. Journal of Molecular Recognition, 2016, 29, 70-79.	1.1	6
17	Quantum Calculations Indicate Effective Electron Transfer between FMN and Benzoquinone in a New Crystal Structure of Escherichia coli WrbA. Journal of Physical Chemistry B, 2016, 120, 4867-4877.	1.2	8
18	Solvation analysis of some Solvatochromic probes in binary mixtures of reline, ethaline, and glyceline with DMSO. Journal of Molecular Liquids, 2016, 222, 845-853.	2.3	38

#	Article	IF	Citations
19	Experimental and Molecular Dynamics Simulation Study of Specific Ion Effect on the Graphene Oxide Surface and Investigation of the Influence on Reactive Extraction of Model Dye Molecule at Waterâ€“Organic Interface. Journal of Physical Chemistry C, 2016, 120, 14088-14100.	1.5	43
20	Molecular dynamics comparison of E. coli WrbA apoprotein and holoprotein. Journal of Molecular Modeling, 2014, 20, 2400.	0.8	1
21	Interdomain communication in the endonuclease/motor subunit of type I restriction-modification enzyme EcoR124I. Journal of Molecular Modeling, 2014, 20, 2334.	0.8	6
22	Binding-competent states for L-arginine in E. coli arginine repressor apoprotein. Journal of Molecular Modeling, 2014, 20, 2330.	0.8	5
23	1.2â€…Ã… resolution crystal structure ofEscherichia coliWrbA holoprotein. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1748-1757.	2.5	6
24	Biphasic Kinetic Behavior of E. coli WrbA, an FMN-Dependent NAD(P)H:Quinone Oxidoreductase. PLoS ONE, 2012, 7, e43902.	1.1	20
25	An in Silico Design for a DNA Nanomechanical Switch. ACS Nano, 2010, 4, 5737-5742.	7.3	13
26	Theoretical Study of the Stability of the DNA Duplexes Modified by a Series of Hydrophobic Base Analogues. Chemistry - A European Journal, 2009, 15, 7601-7610.	1.7	4
27	Potentialâ€Energy and Freeâ€Energy Surfaces of Glycylâ€Phenylalanylâ€Alanine (GFA) Tripeptide: Experiment and Theory. Chemistry - A European Journal, 2008, 14, 4886-4898.	1.7	47
28	A multi-scale method for the calculation of charge transfer rates through the Î-stack of DNA: application to DNA dynamics. Physical Chemistry Chemical Physics, 2008, 10, 5436.	1.3	23
29	Structure of Isolated Tryptophyl-Glycine Dipeptide and Tryptophyl-Glycyl-Glycine Tripeptide:Â Ab Initio SCC-DFTB-D Molecular Dynamics Simulations and High-Level Correlated ab Initio Quantum Chemical Calculations. Journal of Physical Chemistry B, 2006, 110, 6385-6396.	1.2	57
30	Exceptional Thermodynamic Stability of DNA Duplexes Modified by Nonpolar Base Analogues Is due to Increased Stacking Interactions and Favorable Solvation: Correlated Ab Initio Calculations and Molecular Dynamics Simulations. Chemistry - A European Journal, 2006, 12, 3587-3595.	1.7	24
31	Potential Energy Surfaces of an Adenineâ€¯Thymine Base Pair and Its Methylated Analogue in the Presence of One and Two Water Molecules:â€‰ Molecular Mechanics and Correlated Ab Initio Study. Journal of Physical Chemistry B, 2005, 109, 12206-12213.	1.2	33
32	Ferrocene-Modified Purines as Potential Electrochemical Markers: Synthesis, Crystal Structures, Electrochemistry and Cytostatic Activity of (Ferrocenylethynyl)- and (Ferrocenylethyl)purines. Chemistry - A European Journal, 2004, 10, 2058-2066.	1.7	58
33	Origin of Difference between One-Electron Redox Potentials of Guanosine and Guanine:Â Electrochemical and Quantum Chemical Study. Journal of Physical Chemistry B, 2004, 108, 15896-15899.	1.2	22
34	Racemization Barriers of 1,1â€˜-Binaphthyl and 1,1â€˜-Binaphthalene-2,2â€˜-diol:Â A DFT Study. Journal of Organic Chemistry, 2003, 68, 5677-5680.	1.7	132
35	Intercalators. 1. Nature of Stacking Interactions between Intercalators (Ethidium, Daunomycin,) Tj ETQq1 1 0.784314 rgBT /Overlock Functional Theory, and Empirical Potential Study. Journal of the American Chemical Society, 2002, 124, 3366-3376.	6.6	293