

Milan HodoÅ;Äek

List of Publications by Year in descending order

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22
papers

795
citations

1039406

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752256

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docs citations

22
times ranked

1061
citing authors

#	ARTICLE	IF	CITATIONS
1	Automatic Assembly and Calibration of Models of Enzymatic Reactions Based on Ordinary Differential Equations. <i>Methods in Molecular Biology</i> , 2022, 2385, 141-152.	0.4	0
2	Molecular Dynamics Simulations Reveal Interactions of an IgG1 Antibody With Selected Fc Receptors. <i>Frontiers in Chemistry</i> , 2021, 9, 705931.	1.8	4
3	CHARMM Force-Field Parameters for Morphine, Heroin, and Oliceridine, and Conformational Dynamics of Opioid Drugs. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3964-3977.	2.5	8
4	Loop Grafting between Similar Local Environments for Fc-Silent Antibodies. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5475-5486.	2.5	3
5	Potential Energy Function for Fentanyl-Based Opioid Pain Killers. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3566-3576.	2.5	13
6	The redox-coupled proton-channel opening in cytochrome <i>c</i> oxidase. <i>Chemical Science</i> , 2020, 11, 3804-3811.	3.7	6
7	Insight into Inhibitor Binding in the Eukaryotic Proteasome: Computations of the 20S CP. <i>International Journal of Molecular Sciences</i> , 2018, 19, 3858.	1.8	1
8	Simulations of NPC1(NTD):NPC2 Protein Complex Reveal Cholesterol Transfer Pathways. <i>International Journal of Molecular Sciences</i> , 2018, 19, 2623.	1.8	10
9	Role of magnesium ions in the reaction mechanism at the interface between Tm1631 protein and its DNA ligand. <i>Chemistry Central Journal</i> , 2016, 10, 41.	2.6	7
10	Rapid identification of atypical tetracyclines using tandem mass spectrometric fragmentation patterns. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 1556-1562.	0.7	5
11	Efficiently computing pathway free energies: New approaches based on chain-of-replica and Non-Boltzmann Bennett reweighting schemes. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2015, 1850, 944-953.	1.1	28
12	Amino acids as corrosion inhibitors for copper in acidic medium: Experimental and theoretical study. <i>Journal of the Serbian Chemical Society</i> , 2013, 78, 2069-2086.	0.4	25
13	Common Force Field Thermodynamics of Cholesterol. <i>Scientific World Journal</i> , The, 2013, 2013, 1-7.	0.8	1
14	Bound Ligand Conformer Revealed by Flexible Structure Alignment in Absence of Crystal Structures: Indirect Drug Design Probed for HIV-1 Protease Inhibitors. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 659-673.	2.3	0
15	Liquid-Ordered Phase Formation in Cholesterol/Sphingomyelin Bilayers: All-Atom Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 15795-15802.	1.2	46
16	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. <i>Journal of Computational Chemistry</i> , 2007, 28, 1485-1502.	1.5	190
17	Low-lying excited states and photodissociation studies of cis-BrONO. <i>Molecular Physics</i> , 2005, 103, 2375-2380.	0.8	3
18	Exploring the quantum mechanical/molecular mechanical replica path method: a pathway optimization of the chorismate to prephenate Claisen rearrangement catalyzed by chorismate mutase. <i>Theoretical Chemistry Accounts</i> , 2003, 109, 140-148.	0.5	100

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19	CROW for large scale macromolecular simulations. Cellular and Molecular Biology Letters, 2002, 7, 118-9.	2.7	4
20	A Hybrid QM/MM Potential Employing Hartree-Fock or Density Functional Methods in the Quantum Region. Journal of Physical Chemistry A, 1999, 103, 3462-3471.	1.1	155
21	Global Energy Minimization of Small Molecules Combining Constraint Logic Programming and Molecular Mechanics. Journal of Chemical Information and Computer Sciences, 1997, 37, 966-970.	2.8	1
22	Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. Theoretical considerations. International Journal of Quantum Chemistry, 1996, 60, 1189-1200.	1.0	185