Milan HodoÅ¡Äek

List of Publications by Year
in descending order

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22 papers	795 citations	1040056 9 h-index	752698 20 g-index
22 all docs	22 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. Methods in Molecular Biology, 2022, 2385, 141-152.	0.9	0
2	Molecular Dynamics Simulations Reveal Interactions of an IgG1 Antibody With Selected Fc Receptors. Frontiers in Chemistry, 2021, 9, 705931.	3.6	4
3	CHARMM Force-Field Parameters for Morphine, Heroin, and Oliceridine, and Conformational Dynamics of Opioid Drugs. Journal of Chemical Information and Modeling, 2021, 61, 3964-3977.	5.4	8
4	Loop Grafting between Similar Local Environments for Fc-Silent Antibodies. Journal of Chemical Information and Modeling, 2020, 60, 5475-5486.	5.4	3
5	Potential Energy Function for Fentanyl-Based Opioid Pain Killers. Journal of Chemical Information and Modeling, 2020, 60, 3566-3576.	5.4	13
6	The redox-coupled proton-channel opening in cytochrome c oxidase. Chemical Science, 2020, 11, 3804-3811.	7.4	6
7	Insight into Inhibitor Binding in the Eukaryotic Proteasome: Computations of the 20S CP. International Journal of Molecular Sciences, 2018, 19, 3858.	4.1	1
8	Simulations of NPC1(NTD):NPC2 Protein Complex Reveal Cholesterol Transfer Pathways. International Journal of Molecular Sciences, 2018, 19, 2623.	4.1	10
9	Role of magnesium ions in the reaction mechanism at the interface between Tm1631 protein and its DNA ligand. Chemistry Central Journal, 2016, 10, 41.	2.6	7
10	Rapid identification of atypical tetracyclines using tandem mass spectrometric fragmentation patterns. Rapid Communications in Mass Spectrometry, 2015, 29, 1556-1562.	1.5	5
11	Efficiently computing pathway free energies: New approaches based on chain-of-replica and Non-Boltzmann Bennett reweighting schemes. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 944-953.	2.4	28
12	Amino acids as corrosion inhibitors for copper in acidic medium: Experimental and theoretical study. Journal of the Serbian Chemical Society, 2013, 78, 2069-2086.	0.8	25
13	Common Force Field Thermodynamics of Cholesterol. Scientific World Journal, The, 2013, 2013, 1-7.	2.1	1
14	Bound Ligand Conformer Revealed by Flexible Structure Alignment in Absence of Crystal Structures: Indirect Drug Design Probed for HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2009, 5, 659-673.	5.3	0
15	Liquid-Ordered Phase Formation in Cholesterol/Sphingomyelin Bilayers: All-Atom Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 15795-15802.	2.6	46
16	Interfacing Q-Chem and CHARMM to perform QM/MM reaction path calculations. Journal of Computational Chemistry, 2007, 28, 1485-1502.	3.3	190
17	Low-lying excited states and photodissociation studies ofcis-BrONO. Molecular Physics, 2005, 103, 2375-2380.	1.7	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. Theoretical Chemistry Accounts, 2003, 109, 140-148.	1.4	100

#	Article	IF	Citations
19	CROW for large scale macromolecular simulations. Cellular and Molecular Biology Letters, 2002, 7, 118-9.	7.0	4
20	A Hybrid QMâ˜'MM Potential Employing Hartreeâ˜'Fock or Density Functional Methods in the Quantum Region. Journal of Physical Chemistry A, 1999, 103, 3462-3471.	2.5	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.	2.0	185