

List of Publications by Year in descending order

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20
papers

14,444
citations

448610

19
h-index

889612

19
g-index

21
all docs

21
docs citations

21
times ranked

17792
citing authors

#	ARTICLE	IF	CITATIONS
1	The Amber biomolecular simulation programs. <i>Journal of Computational Chemistry</i> , 2005, 26, 1668-1688.	1.5	7,742
2	Exploring protein native states and large-scale conformational changes with a modified generalized born model. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 383-394.	1.5	2,068
3	H++: a server for estimating pKas and adding missing hydrogens to macromolecules. <i>Nucleic Acids Research</i> , 2005, 33, W368-W371.	6.5	1,295
4	Modification of the Generalized Born Model Suitable for Macromolecules. <i>Journal of Physical Chemistry B</i> , 2000, 104, 3712-3720.	1.2	973
5	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. <i>Journal of Computational Chemistry</i> , 2004, 25, 265-284.	1.5	523
6	Effective Born radii in the generalized Born approximation: The importance of being perfect. <i>Journal of Computational Chemistry</i> , 2002, 23, 1297-1304.	1.5	412
7	Generalized Born Model with a Simple, Robust Molecular Volume Correction. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 156-169.	2.3	334
8	A simple clustering algorithm can be accurate enough for use in calculations of pKs in macromolecules. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 63, 928-938.	1.5	270
9	A Novel View of pH Titration in Biomolecules. <i>Biochemistry</i> , 2001, 40, 3413-3419.	1.2	183
10	Analytical electrostatics for biomolecules: Beyond the generalized Born approximation. <i>Journal of Chemical Physics</i> , 2006, 124, 124902.	1.2	113
11	Incorporating variable dielectric environments into the generalized Born model. <i>Journal of Chemical Physics</i> , 2005, 122, 094511.	1.2	82
12	Implicit Solvent Models in Molecular Dynamics Simulations: A Brief Overview. <i>Annual Reports in Computational Chemistry</i> , 2008, 4, 125-137.	0.9	82
13	A Computational Study of Nucleosomal DNA Flexibility. <i>Biophysical Journal</i> , 2006, 91, 4121-4132.	0.2	72
14	Proton Affinity Changes Driving Unidirectional Proton Transport in the Bacteriorhodopsin Photocycle. <i>Journal of Molecular Biology</i> , 2003, 332, 1183-1193.	2.0	63
15	Analysis of integral expressions for effective Born radii. <i>Journal of Chemical Physics</i> , 2007, 127, 185101.	1.2	54
16	Structural Details, Pathways, and Energetics of Unfolding Apomyoglobin. <i>Journal of Molecular Biology</i> , 2003, 325, 555-567.	2.0	52
17	Analysis of Basic Clustering Algorithms for Numerical Estimation of Statistical Averages in Biomolecules. <i>Journal of Computational Biology</i> , 2008, 15, 165-184.	0.8	39
18	An analytical approach to computing biomolecular electrostatic potential. I. Derivation and analysis. <i>Journal of Chemical Physics</i> , 2008, 129, 075101.	1.2	27

#	ARTICLE	IF	CITATIONS
19	An analytical approach to computing biomolecular electrostatic potential. II. Validation and applications. Journal of Chemical Physics, 2008, 129, 075102.	1.2	27
20	Multiscale Approximation with Graphical Processing Units for Multiplicative Speedup in Molecular Dynamics. , 2016, , .		0