

# Dhruva K Chakravorty

## List of Publications by Year in descending order

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17  
papers

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citations

840119

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1457  
citing authors

#	ARTICLE	IF	CITATIONS
1	Rational Design of Particle Mesh Ewald Compatible Lennard-Jones Parameters for +2 Metal Cations in Explicit Solvent. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2733-2748.	2.3	559
2	Insight into the Cation $\pi$ Interaction at the Metal Binding Site of the Copper Metallochaperone CusF. <i>Journal of the American Chemical Society</i> , 2011, 133, 19330-19333.	6.6	53
3	Solution Structure of <i>Mycobacterium tuberculosis</i> NmtR in the Apo State: Insights into Ni(II)-Mediated Allostery. <i>Biochemistry</i> , 2012, 51, 2619-2629.	1.2	42
4	Simulations of Allosteric Motions in the Zinc Sensor CzrA. <i>Journal of the American Chemical Society</i> , 2012, 134, 3367-3376.	6.6	42
5	Hybrid Quantum/Classical Molecular Dynamics Simulations of the Proton Transfer Reactions Catalyzed by Ketosteroid Isomerase: Analysis of Hydrogen Bonding, Conformational Motions, and Electrostatics. <i>Biochemistry</i> , 2009, 48, 10608-10619.	1.2	37
6	Impact of Mutation on Proton Transfer Reactions in Ketosteroid Isomerase: Insights from Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2010, 132, 7549-7555.	6.6	32
7	Finding a Needle in the Haystack: Computational Modeling of Mg <sup>2+</sup> Binding in the Active Site of Protein Farnesyltransferase. <i>Biochemistry</i> , 2010, 49, 9658-9666.	1.2	27
8	Structure and Dynamics of the N-Terminal Domain of the Cu(I) Binding Protein CusB. <i>Biochemistry</i> , 2013, 52, 6911-6923.	1.2	26
9	Energetics of Zinc-Mediated Interactions in the Allosteric Pathways of Metal Sensor Proteins. <i>Journal of the American Chemical Society</i> , 2013, 135, 30-33.	6.6	24
10	Solution NMR refinement of a metal ion bound protein using metal ion inclusive restrained molecular dynamics methods. <i>Journal of Biomolecular NMR</i> , 2013, 56, 125-137.	1.6	22
11	Implementation of Umbrella Integration within the Framework of the Empirical Valence Bond Approach. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1974-1980.	2.3	15
12	Characterizing Solution Surface Loop Conformational Flexibility of the GM2 Activator Protein. <i>Journal of Physical Chemistry B</i> , 2014, 118, 10607-10617.	1.2	12
13	Role of Substrate Dynamics in Protein Prenylation Reactions. <i>Accounts of Chemical Research</i> , 2015, 48, 439-448.	7.6	11
14	Models for the Metal Transfer Complex of the N-Terminal Region of CusB and CusF. <i>Biochemistry</i> , 2015, 54, 4226-4235.	1.2	10
15	Studying Allosteric Regulation in Metal Sensor Proteins Using Computational Methods. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 181-218.	1.0	9
16	Metal Ion Capture Mechanism of a Copper Metallochaperone. <i>Biochemistry</i> , 2016, 55, 501-509.	1.2	9
17	A combined cheminformatic and bioinformatic approach to address the proteolytic stability challenge in peptide-based drug discovery. <i>Biopolymers</i> , 2015, 104, 775-789.	1.2	2