Shuanghong Huo

List of Publications by Year
in descending order

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34 papers	5,439 citations	430442 18 h-index	395343 33 g-index
36 all docs	36 docs citations	36 times ranked	6546 citing authors

#	Article	IF	Citations
1	Calculating Structures and Free Energies of Complex Molecules:â€‰ Combining Molecular Mechanics and Continuum Models. Accounts of Chemical Research, 2000, 33, 889-897.	7.6	4,098
2	Computational alanine scanning of the 1:1 human growth hormone-receptor complex. Journal of Computational Chemistry, 2002, 23, 15-27.	1.5	288
3	Molecular Dynamics and Free Energy Analyses of Cathepsin Dâ^'Inhibitor Interactions:â€‰ Insight into Structure-Based Ligand Design. Journal of Medicinal Chemistry, 2002, 45, 1412-1419.	2.9	168
4	The MaxFlux algorithm for calculating variationally optimized reaction paths for conformational transitions in many body systems at finite temperature. Journal of Chemical Physics, 1997, 107, 5000-5006.	1.2	122
5	Solvation Model Based on Weighted Solvent Accessible Surface Area. Journal of Physical Chemistry B, 2001, 105, 5055-5067.	1.2	107
6	Formation and Growth of Oligomers: A Monte Carlo Study of an Amyloid Tau Fragment. PLoS Computational Biology, 2008, 4, e1000238.	1.5	104
7	A Novel Mutant Cardiac Troponin C Disrupts Molecular Motions Critical for Calcium Binding Affinity and Cardiomyocyte Contractility. Biophysical Journal, 2008, 94, 3577-3589.	0.2	62
8	Long Time Dynamic Simulations:â€‰ Exploring the Folding Pathways of an Alzheimer's Amyloid AÎ²-Peptide. Accounts of Chemical Research, 2002, 35, 473-481.	7.6	59
9	Molecular Dynamics Simulation Study of the B-States of Solvated Carbon Monoxymyoglobin. Journal of the American Chemical Society, 1997, 119, 2541-2551.	6.6	51
10	Direct computation of long time processes in peptides and proteins: Reaction path study of the coil-to-helix transition in polyalanine. Proteins: Structure, Function and Bioinformatics, 1999, 36, 249-261.	1.5	47
11	Why is Leu55â†'Pro55 transthyretin variant the most amyloidogenic: Insights from molecular dynamics simulations of transthyretin monomers. Protein Science, 2003, 12, 1222-1231.	3.1	43
12	Evaluation of Dimensionality-Reduction Methods from Peptide Foldingâ€“Unfolding Simulations. Journal of Chemical Theory and Computation, 2013, 9, 2490-2497.	2.3	34
13	Conformations of Islet Amyloid Polypeptide Monomers in a Membrane Environment: Implications for Fibril Formation. PLoS ONE, 2012, 7, e47150.	1.1	30
14	The Sequence-Dependent Unfolding Pathway Plays a Critical Role in the Amyloidogenicity of Transthyretinâ€. Biochemistry, 2006, 45, 11992-12002.	1.2	28
15	Initial Conformational Changes of Human Transthyretin under Partially Denaturing Conditions. Biophysical Journal, 2005, 89, 433-443.	0.2	26
16	Evaluation of Configurational Entropy Methods from Peptide Foldingâ^'Unfolding Simulation. Journal of Physical Chemistry B, 2007, 111, 13807-13813.	1.2	25
17	Structural and Pathway Complexity of Î²-Strand Reorganization within Aggregates of Human Transthyretin(105â^'115) Peptide. Journal of Physical Chemistry B, 2007, 111, 5425-5433.	1.2	21
18	Intrinsic versus mutation dependent instability/flexibility: a comparative analysis of the structure and dynamics of wild-type transthyretin and its pathogenic variants. Journal of Structural Biology, 2004, 148, 153-168.	1.3	20

#	Article	IF	Citations
19	Peptide Plane Can Flip in Two Opposite Directions:Â Implication in Amyloid Formation of Transthyretin. Journal of Physical Chemistry B, 2006, 110, 5829-5833.	1.2	18
20	Temperature-Dependent Probabilistic Roadmap Algorithm for Calculating Variationally Optimized Conformational Transition Pathways. Journal of Chemical Theory and Computation, 2007, 3, 17-25.	2.3	14
21	Predicting the Folding Pathway of Engrailed Homeodomain with a Probabilistic Roadmap Enhanced Reaction-Path Algorithm. Biophysical Journal, 2008, 94, 1622-1629.	0.2	11
22	Quantum mechanical studies on model Î±â€pleated sheets. Journal of Computational Chemistry, 2010, 31, 1216-1223.	1.5	10
23	Observation of Two Families of Folding Pathways of BBL. Biophysical Journal, 2011, 100, 2457-2465.	0.2	9
24	Graph representation of protein free energy landscape. Journal of Chemical Physics, 2013, 139, 185101.	1.2	8
25	Network representation of conformational transitions between hidden intermediates of Rd-apocytochrome b562. Journal of Chemical Physics, 2015, 143, 135101.	1.2	6
26	Potential influence of Asp in the Ca2+ coordination position 5 of parvalbumin on the calcium-binding affinity: A computational study. Journal of Inorganic Biochemistry, 2006, 100, 1879-1887.	1.5	5
27	Euclidean sections of protein conformation space and their implications in dimensionality reduction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2585-2596.	1.5	5
28	Effects of Two Solvent Conditions on the Free Energy Landscape of the BBL Peripheral Subunit Binding Domain. Journal of Physical Chemistry B, 2012, 116, 646-652.	1.2	4
29	Observations on AMBER Force Field Performance under the Conditions of Low pH and High Salt Concentrations. Journal of Physical Chemistry B, 2017, 121, 9838-9847.	1.2	4
30	Long-Range Reactivity Modulations in Geranyl Chloride Derivatives. Journal of Organic Chemistry, 2016, 81, 10964-10974.	1.7	3
31	Interplay between human islet amyloid polypeptide aggregates and micro-heterogeneous membranes. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183691.	1.4	3
32	Direct computation of long time processes in peptides and proteins: Reaction path study of the coil-to-helix transition in polyalanine. , 1999, 36, 249.		3
33	Inherent structure versus geometric metric for state space discretization. Journal of Computational Chemistry, 2016, 37, 1251-1258.	1.5	2
34	Approximating dynamic proximity with a hybrid geometry energy-based kernel for diffusion maps. Journal of Chemical Physics, 2019, 151, 105101.	1.2	1