

Donald J Jacobs

List of Publications by Year in descending order

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52
papers

2,525
citations

394421
19
h-index

223800
46
g-index

53
all docs

53
docs citations

53
times ranked

2460
citing authors

#	ARTICLE	IF	CITATIONS
1	Principal Component Analysis: A Method for Determining the Essential Dynamics of Proteins. <i>Methods in Molecular Biology</i> , 2014, 1084, 193-226.	0.9	677
2	Protein flexibility predictions using graph theory. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 44, 150-165.	2.6	670
3	An Algorithm for Two-Dimensional Rigidity Percolation: The Pebble Game. <i>Journal of Computational Physics</i> , 1997, 137, 346-365.	3.8	294
4	Conserved quantitative stability/flexibility relationships (QSFR) in an orthologous RNase H pair. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 130-143.	2.6	54
5	Elucidating Protein Thermodynamics from the Three-Dimensional Structure of the Native State Using Network Rigidity. <i>Biophysical Journal</i> , 2005, 88, 903-915.	0.5	53
6	New insight into long-range nonadditivity within protein double-mutant cycles. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 915-924.	2.6	52
7	Network rigidity at finite temperature: Relationships between thermodynamic stability, the nonadditivity of entropy, and cooperativity in molecular systems. <i>Physical Review E</i> , 2003, 68, 061109.	2.1	50
8	Hydrogen bond networks determine emergent mechanical and thermodynamic properties across a protein family. <i>Chemistry Central Journal</i> , 2008, 2, 17.	2.6	44
9	Changes in Lysozyme Flexibility upon Mutation Are Frequent, Large and Long-Ranged. <i>PLoS Computational Biology</i> , 2012, 8, e1002409.	3.2	42
10	Elucidating Quantitative Stability/Flexibility Relationships Within Thioredoxin and its Fragments Using a Distance Constraint Model. <i>Journal of Molecular Biology</i> , 2006, 358, 882-904.	4.2	39
11	Rigidity Emerges during Antibody Evolution in Three Distinct Antibody Systems: Evidence from QSFR Analysis of Fab Fragments. <i>PLoS Computational Biology</i> , 2015, 11, e1004327.	3.2	39
12	Redistribution of Flexibility in Stabilizing Antibody Fragment Mutants Follows Le Chatelier's Principle. <i>PLoS ONE</i> , 2014, 9, e92870.	2.5	37
13	Allosteric Response Is both Conserved and Variable across Three CheY Orthologs. <i>Biophysical Journal</i> , 2010, 99, 2245-2254.	0.5	32
14	Unifying mechanical and thermodynamic descriptions across the thioredoxin protein family. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 610-627.	2.6	31
15	Understanding the α -helix to coil transition in polypeptides using network rigidity: Predicting heat and cold denaturation in mixed solvent conditions. <i>Biopolymers</i> , 2004, 75, 1-31.	2.4	27
16	Kinetics and Thermodynamics of the Rate-Limiting Conformational Change in the Actomyosin V Mechanochemical Cycle. <i>Journal of Molecular Biology</i> , 2011, 407, 716-730.	4.2	27
17	Statistical Measures to Quantify Similarity between Molecular Dynamics Simulation Trajectories. <i>Entropy</i> , 2017, 19, 646.	2.2	27
18	Conformational Entropy of an Ideal Cross-Linking Polymer Chain. <i>Entropy</i> , 2008, 10, 285-308.	2.2	26

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19	Switch II Mutants Reveal Coupling between the Nucleotide- and Actin-Binding Regions in Myosin V. Biophysical Journal, 2012, 102, 2545-2555.	0.5	25
20	Helix/Coil Nucleation: A Local Response to Global Demands. Biophysical Journal, 2009, 97, 3000-3009.	0.5	22
21	Ensemble Properties of Network Rigidity Reveal Allosteric Mechanisms. Methods in Molecular Biology, 2012, 796, 279-304.	0.9	21
22	Variations within Class-A β -Lactamase Physiochemical Properties Reflect Evolutionary and Environmental Patterns, but not Antibiotic Specificity. PLoS Computational Biology, 2013, 9, e1003155.	3.2	19
23	Nonadditivity in Conformational Entropy upon Molecular Rigidification Reveals a Universal Mechanism Affecting Folding Cooperativity. Biophysical Journal, 2011, 100, 1129-1138.	0.5	18
24	Decomposing Dynamical Couplings in Mutated scFv Antibody Fragments into Stabilizing and Destabilizing Effects. Journal of the American Chemical Society, 2017, 139, 17508-17517.	13.7	18
25	Ensemble-based methods for describing protein dynamics. Current Opinion in Pharmacology, 2010, 10, 760-769.	3.5	17
26	Predicting the Melting Point of Human C-Type Lysozyme Mutants. Current Protein and Peptide Science, 2010, 11, 562-572.	1.4	15
27	Thermodynamic Stability and Flexibility Characteristics of Antibody Fragment Complexes. Protein and Peptide Letters, 2013, 21, 752-765.	0.9	14
28	Dynamics and thermodynamic properties of CXCL7 chemokine. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1987-2007.	2.6	13
29	High throughput nonparametric probability density estimation. PLoS ONE, 2018, 13, e0196937.	2.5	13
30	Mutations in Antibody Fragments Modulate Allosteric Response Via Hydrogen-Bond Network Fluctuations. Biophysical Journal, 2016, 110, 1933-1942.	0.5	11
31	JED: a Java Essential Dynamics Program for comparative analysis of protein trajectories. BMC Bioinformatics, 2017, 18, 271.	2.6	11
32	Molecular function recognition by supervised projection pursuit machine learning. Scientific Reports, 2021, 11, 4247.	3.3	10
33	A Case Study Comparing Quantitative Stability-Flexibility Relationships Across Five Metallo- β -Lactamases Highlighting Differences Within NDM-1. Methods in Molecular Biology, 2014, 1084, 227-238.	0.9	10
34	Elucidating the Conformational Dependence of Calculated pKa Values. Journal of Chemical Theory and Computation, 2006, 2, 927-938.	5.3	8
35	Novel Ricin Subunit Antigens With Enhanced Capacity to Elicit Toxin-Neutralizing Antibody Responses in Mice. Journal of Pharmaceutical Sciences, 2016, 105, 1603-1613.	3.3	8
36	Nonadditivity in the α -helix to coil transition. Biopolymers, 2011, 95, 240-253.	2.4	7

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37	Calculating Ensemble Averaged Descriptions of Protein Rigidity without Sampling. PLoS ONE, 2012, 7, e29176.	2.5	7
38	Best Probability Density Function for Random Sampled Data. Entropy, 2009, 11, 1001-1024.	2.2	6
39	WaveMap: Interactively Discovering Features From Protein Flexibility Matrices Using Wavelet-based Visual Analytics. Computer Graphics Forum, 2011, 30, 1001-1010.	3.0	6
40	Universal Sample Size Invariant Measures for Uncertainty Quantification in Density Estimation. Entropy, 2019, 21, 1120.	2.2	5
41	MATLAB tool for probability density assessment and nonparametric estimation. SoftwareX, 2022, 18, 101017.	2.6	5
42	A Signal Processing Method to Explore Similarity in Protein Flexibility. Advances in Bioinformatics, 2010, 2010, 1-8.	5.7	3
43	A visual analytics approach to exploring protein flexibility subspaces. , 2013, , .		3
44	JEDi: java essential dynamics inspector – a molecular trajectory analysis toolkit. BMC Bioinformatics, 2021, 22, 226.	2.6	3
45	Functional Dynamics of Substrate Recognition in TEM Beta-Lactamase. Entropy, 2022, 24, 729.	2.2	2
46	A virtual pebble game to ensemble average graph rigidity. Algorithms for Molecular Biology, 2015, 10, 11.	1.2	1
47	Molecular clustering and percolation characteristics near the glass transition in aqueous trehalose and choline dihydrogen phosphate solutions. Physical Chemistry Chemical Physics, 2018, 20, 20899-20909.	2.8	1
48	Rigidity and flexibility characteristics of DD[E/D]-transposases Mos1 and Sleeping Beauty. Proteins: Structure, Function and Bioinformatics, 2019, 87, 313-325.	2.6	1
49	Biased Hypothesis Formation From Projection Pursuit. , 2021, 01, 221-233.		1
50	Towards Comprehensive Analysis of Protein Family Quantitative Stability-Flexibility Relationships Using Homology Models. Methods in Molecular Biology, 2014, 1084, 239-254.	0.9	0
51	Victory Tax: A Holistic Income Tax System. Entropy, 2021, 23, 1492.	2.2	0
52	Classifying EEG motor imagery signals using supervised projection pursuit for artefact removal. , 2021, , .		0