Donald J Jacobs

List of Publications by Year
in descending order

52	2,525	393982	223531
papers	citations	19 h-index	46 g-index

53	53	53	2460
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	MATLAB tool for probability density assessment and nonparametric estimation. SoftwareX, 2022, 18, 101017.	1.2	5
2	Functional Dynamics of Substrate Recognition in TEM Beta-Lactamase. Entropy, 2022, 24, 729.	1.1	2
3	Molecular function recognition by supervised projection pursuit machine learning. Scientific Reports, 2021, 11, 4247.	1.6	10
4	JEDi: java essential dynamics inspector â€" a molecular trajectory analysis toolkit. BMC Bioinformatics, 2021, 22, 226.	1.2	3
5	Victory Tax: A Holistic Income Tax System. Entropy, 2021, 23, 1492.	1.1	0
6	Biased Hypothesis Formation From Projection Pursuit. , 2021, 01, 221-233.		1
7	Classifying EEG motor imagery signals using supervised projection pursuit for artefact removal. , 2021, , .		0
8	Universal Sample Size Invariant Measures for Uncertainty Quantification in Density Estimation. Entropy, 2019, 21, 1120.	1.1	5
9	Rigidity and flexibility characteristics of DD[E/D]â€transposases Mos1 and Sleeping Beauty. Proteins: Structure, Function and Bioinformatics, 2019, 87, 313-325.	1.5	1
10	High throughput nonparametric probability density estimation. PLoS ONE, 2018, 13, e0196937.	1.1	13
11	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.	1.3	1
12	Decomposing Dynamical Couplings in Mutated scFv Antibody Fragments into Stabilizing and Destabilizing Effects. Journal of the American Chemical Society, 2017, 139, 17508-17517.	6.6	18
13	JED: a Java Essential Dynamics Program for comparative analysis of protein trajectories. BMC Bioinformatics, 2017, 18, 271.	1.2	11
14	Statistical Measures to Quantify Similarity between Molecular Dynamics Simulation Trajectories. Entropy, 2017, 19, 646.	1.1	27
15	Mutations in Antibody Fragments Modulate Allosteric Response Via Hydrogen-Bond Network Fluctuations. Biophysical Journal, 2016, 110, 1933-1942.	0.2	11
16	Novel Ricin Subunit Antigens With Enhanced Capacity to Elicit Toxin-Neutralizing Antibody Responses in Mice. Journal of Pharmaceutical Sciences, 2016, 105, 1603-1613.	1.6	8
17	Dynamics and thermodynamic properties of CXCL7 chemokine. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1987-2007.	1.5	13
18	Rigidity Emerges during Antibody Evolution in Three Distinct Antibody Systems: Evidence from QSFR Analysis of Fab Fragments. PLoS Computational Biology, 2015, 11, e1004327.	1.5	39

#	Article	IF	Citations
19	A virtual pebble game to ensemble average graph rigidity. Algorithms for Molecular Biology, 2015, 10, 11.	0.3	1
20	Redistribution of Flexibility in Stabilizing Antibody Fragment Mutants Follows Le ChÃ¢telierâ€™s Principle. PLoS ONE, 2014, 9, e92870.	1.1	37
21	Principal Component Analysis: A Method for Determining the Essential Dynamics of Proteins. Methods in Molecular Biology, 2014, 1084, 193-226.	0.4	677
22	A Case Study Comparing Quantitative Stabilityâ€“Flexibility Relationships Across Five Metallo-Î²-Lactamases Highlighting Differences Within NDM-1. Methods in Molecular Biology, 2014, 1084, 227-238.	0.4	10
23	Towards Comprehensive Analysis of Protein Family Quantitative Stabilityâ€“Flexibility Relationships Using Homology Models. Methods in Molecular Biology, 2014, 1084, 239-254.	0.4	0
24	Variations within Class-A Î²-Lactamase Physiochemical Properties Reflect Evolutionary and Environmental Patterns, but not Antibiotic Specificity. PLoS Computational Biology, 2013, 9, e1003155.	1.5	19
25	A visual analytics approach to exploring protein flexibility subspaces. , 2013, , .		3
26	Thermodynamic Stability and Flexibility Characteristics of Antibody Fragment Complexes. Protein and Peptide Letters, 2013, 21, 752-765.	0.4	14
27	Changes in Lysozyme Flexibility upon Mutation Are Frequent, Large and Long-Ranged. PLoS Computational Biology, 2012, 8, e1002409.	1.5	42
28	Switch II Mutants Reveal Coupling between the Nucleotide- and Actin-Binding Regions in Myosin V. Biophysical Journal, 2012, 102, 2545-2555.	0.2	25
29	Ensemble Properties of Network Rigidity Reveal Allosteric Mechanisms. Methods in Molecular Biology, 2012, 796, 279-304.	0.4	21
30	Calculating Ensemble Averaged Descriptions of Protein Rigidity without Sampling. PLoS ONE, 2012, 7, e29176.	1.1	7
31	Nonadditivity in Conformational Entropy upon Molecular Rigidification Reveals a Universal Mechanism Affecting Folding Cooperativity. Biophysical Journal, 2011, 100, 1129-1138.	0.2	18
32	Kinetics and Thermodynamics of the Rate-Limiting Conformational Change in the Actomyosin V Mechanochemical Cycle. Journal of Molecular Biology, 2011, 407, 716-730.	2.0	27
33	WaveMap: Interactively Discovering Features From Protein Flexibility Matrices Using Waveletâ€based Visual Analytics. Computer Graphics Forum, 2011, 30, 1001-1010.	1.8	6
34	Nonadditivity in the alphaâ€helix to coil transition. Biopolymers, 2011, 95, 240-253.	1.2	7
35	A Signal Processing Method to Explore Similarity in Protein Flexibility. Advances in Bioinformatics, 2010, 2010, 1-8.	5.7	3
36	Predicting the Melting Point of Human C-Type Lysozyme Mutants. Current Protein and Peptide Science, 2010, 11, 562-572.	0.7	15

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37	Allosteric Response Is both Conserved and Variable across Three CheY Orthologs. Biophysical Journal, 2010, 99, 2245-2254.	0.2	32
38	Ensemble-based methods for describing protein dynamics. Current Opinion in Pharmacology, 2010, 10, 760-769.	1.7	17
39	Best Probability Density Function for Random Sampled Data. Entropy, 2009, 11, 1001-1024.	1.1	6
40	Unifying mechanical and thermodynamic descriptions across the thioredoxin protein family. Proteins: Structure, Function and Bioinformatics, 2009, 75, 610-627.	1.5	31
41	Helix/Coil Nucleation: A Local Response to Global Demands. Biophysical Journal, 2009, 97, 3000-3009.	0.2	22
42	Hydrogen bond networks determine emergent mechanical and thermodynamic properties across a protein family. Chemistry Central Journal, 2008, 2, 17.	2.6	44
43	New insight into longâ€range nonadditivity within protein doubleâ€mutant cycles. Proteins: Structure, Function and Bioinformatics, 2008, 70, 915-924.	1.5	52
44	Conformational Entropy of an Ideal Cross-Linking Polymer Chain. Entropy, 2008, 10, 285-308.	1.1	26
45	Elucidating the Conformational Dependence of Calculated pKa Values. Journal of Chemical Theory and Computation, 2006, 2, 927-938.	2.3	8
46	Elucidating Quantitative Stability/Flexibility Relationships Within Thioredoxin and its Fragments Using a Distance Constraint Model. Journal of Molecular Biology, 2006, 358, 882-904.	2.0	39
47	Conserved quantitative stability/flexibility relationships (QSFR) in an orthologous RNase H pair. Proteins: Structure, Function and Bioinformatics, 2005, 62, 130-143.	1.5	54
48	Elucidating Protein Thermodynamics from the Three-Dimensional Structure of the Native State Using Network Rigidity. Biophysical Journal, 2005, 88, 903-915.	0.2	53
49	Understanding the ?-helix to coil transition in polypeptides using network rigidity: Predicting heat and cold denaturation in mixed solvent conditions. Biopolymers, 2004, 75, 1-31.	1.2	27
50	Network rigidity at finite temperature: Relationships between thermodynamic stability, the nonadditivity of entropy, and cooperativity in molecular systems. Physical Review E, 2003, 68, 061109.	0.8	50
51	Protein flexibility predictions using graph theory. Proteins: Structure, Function and Bioinformatics, 2001, 44, 150-165.	1.5	670
52	An Algorithm for Two-Dimensional Rigidity Percolation: The Pebble Game. Journal of Computational Physics, 1997, 137, 346-365.	1.9	294