

# Donald J Jacobs

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/1298192/publications.pdf>

Version: 2024-02-01

52  
papers

2,525  
citations

393982

19  
h-index

223531

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.	0.4	677
2	Protein flexibility predictions using graph theory. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 44, 150-165.	1.5	670
3	An Algorithm for Two-Dimensional Rigidity Percolation: The Pebble Game. <i>Journal of Computational Physics</i> , 1997, 137, 346-365.	1.9	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.	1.5	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.	0.2	53
6	New insight into long-range nonadditivity within protein double mutant cycles. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 915-924.	1.5	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.	0.8	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.	1.5	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.	2.0	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.	1.5	39
12	Redistribution of Flexibility in Stabilizing Antibody Fragment Mutants Follows Le Chatelier's Principle. <i>PLoS ONE</i> , 2014, 9, e92870.	1.1	37
13	Allosteric Response Is both Conserved and Variable across Three CheY Orthologs. <i>Biophysical Journal</i> , 2010, 99, 2245-2254.	0.2	32
14	Unifying mechanical and thermodynamic descriptions across the thioredoxin protein family. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 75, 610-627.	1.5	31
15	Understanding the $\alpha$ -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.	1.2	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.	2.0	27
17	Statistical Measures to Quantify Similarity between Molecular Dynamics Simulation Trajectories. <i>Entropy</i> , 2017, 19, 646.	1.1	27
18	Conformational Entropy of an Ideal Cross-Linking Polymer Chain. <i>Entropy</i> , 2008, 10, 285-308.	1.1	26

#	ARTICLE	IF	CITATIONS
19	Switch II Mutants Reveal Coupling between the Nucleotide- and Actin-Binding Regions in Myosin V. <i>Biophysical Journal</i> , 2012, 102, 2545-2555.	0.2	25
20	Helix/Coil Nucleation: A Local Response to Global Demands. <i>Biophysical Journal</i> , 2009, 97, 3000-3009.	0.2	22
21	Ensemble Properties of Network Rigidity Reveal Allosteric Mechanisms. <i>Methods in Molecular Biology</i> , 2012, 796, 279-304.	0.4	21
22	Variations within Class-A $\beta$ -Lactamase Physicochemical Properties Reflect Evolutionary and Environmental Patterns, but not Antibiotic Specificity. <i>PLoS Computational Biology</i> , 2013, 9, e1003155.	1.5	19
23	Nonadditivity in Conformational Entropy upon Molecular Rigidification Reveals a Universal Mechanism Affecting Folding Cooperativity. <i>Biophysical Journal</i> , 2011, 100, 1129-1138.	0.2	18
24	Decomposing Dynamical Couplings in Mutated scFv Antibody Fragments into Stabilizing and Destabilizing Effects. <i>Journal of the American Chemical Society</i> , 2017, 139, 17508-17517.	6.6	18
25	Ensemble-based methods for describing protein dynamics. <i>Current Opinion in Pharmacology</i> , 2010, 10, 760-769.	1.7	17
26	Predicting the Melting Point of Human C-Type Lysozyme Mutants. <i>Current Protein and Peptide Science</i> , 2010, 11, 562-572.	0.7	15
27	Thermodynamic Stability and Flexibility Characteristics of Antibody Fragment Complexes. <i>Protein and Peptide Letters</i> , 2013, 21, 752-765.	0.4	14
28	Dynamics and thermodynamic properties of CXCL7 chemokine. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 1987-2007.	1.5	13
29	High throughput nonparametric probability density estimation. <i>PLoS ONE</i> , 2018, 13, e0196937.	1.1	13
30	Mutations in Antibody Fragments Modulate Allosteric Response Via Hydrogen-Bond Network Fluctuations. <i>Biophysical Journal</i> , 2016, 110, 1933-1942.	0.2	11
31	JED: a Java Essential Dynamics Program for comparative analysis of protein trajectories. <i>BMC Bioinformatics</i> , 2017, 18, 271.	1.2	11
32	Molecular function recognition by supervised projection pursuit machine learning. <i>Scientific Reports</i> , 2021, 11, 4247.	1.6	10
33	A Case Study Comparing Quantitative Stability-Flexibility Relationships Across Five Metallo- $\beta$ -Lactamases Highlighting Differences Within NDM-1. <i>Methods in Molecular Biology</i> , 2014, 1084, 227-238.	0.4	10
34	Elucidating the Conformational Dependence of Calculated pKa Values. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 927-938.	2.3	8
35	Novel Ricin Subunit Antigens With Enhanced Capacity to Elicit Toxin-Neutralizing Antibody Responses in Mice. <i>Journal of Pharmaceutical Sciences</i> , 2016, 105, 1603-1613.	1.6	8
36	Nonadditivity in the $\alpha$ -helix to coil transition. <i>Biopolymers</i> , 2011, 95, 240-253.	1.2	7

#	ARTICLE	IF	CITATIONS
37	Calculating Ensemble Averaged Descriptions of Protein Rigidity without Sampling. PLoS ONE, 2012, 7, e29176.	1.1	7
38	Best Probability Density Function for Random Sampled Data. Entropy, 2009, 11, 1001-1024.	1.1	6
39	WaveMap: Interactively Discovering Features From Protein Flexibility Matrices Using Wavelet-based Visual Analytics. Computer Graphics Forum, 2011, 30, 1001-1010.	1.8	6
40	Universal Sample Size Invariant Measures for Uncertainty Quantification in Density Estimation. Entropy, 2019, 21, 1120.	1.1	5
41	MATLAB tool for probability density assessment and nonparametric estimation. SoftwareX, 2022, 18, 101017.	1.2	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.	1.2	3
45	Functional Dynamics of Substrate Recognition in TEM Beta-Lactamase. Entropy, 2022, 24, 729.	1.1	2
46	A virtual pebble game to ensemble average graph rigidity. Algorithms for Molecular Biology, 2015, 10, 11.	0.3	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.	1.3	1
48	Rigidity and flexibility characteristics of DD[E/D]-transposases Mos1 and Sleeping Beauty. Proteins: Structure, Function and Bioinformatics, 2019, 87, 313-325.	1.5	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.	0.4	0
51	Victory Tax: A Holistic Income Tax System. Entropy, 2021, 23, 1492.	1.1	0
52	Classifying EEG motor imagery signals using supervised projection pursuit for artefact removal. , 2021, , .		0