Steven Hayward

List of Publications by Year in descending order

52 papers	3,256 citations	304743 22 h-index	206112 48 g-index
52 all docs	52 docs citations	52 times ranked	3547 citing authors

#	Article	IF	Citations
1	Determination of amino acids that favour the Î±L region using Ramachandran propensity plots. Implications for Î±-sheet as the possible amyloid intermediate. Journal of Structural Biology, 2021, 213, 107738.	2.8	7
2	The role of the half-turn in determining structures of Alzheimerâ€™s AÎ² wild-type and mutants. Journal of Structural Biology, 2021, 213, 107792.	2.8	1
3	DockIT: a tool for interactive molecular docking and molecular complex construction. Bioinformatics, 2021, 36, 5698-5700.	4.1	7
4	Investigation of sequence features of hinge-bending regions in proteins with domain movements using kernel logistic regression. BMC Bioinformatics, 2020, 21, 137.	2.6	3
5	Multi-strand Î²-sheet of Alzheimer AÎ²(1â€“40) folds to Î²-strip helix: implication for protofilament formation. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2143-2153.	3.5	1
6	Haptic-Assisted Interactive Molecular Docking Incorporating Receptor Flexibility. Journal of Chemical Information and Modeling, 2019, 59, 2900-2912.	5.4	15
7	Free Energy Profile of Domain Movement in Ligand-Free Citrate Synthase. Journal of Physical Chemistry B, 2019, 123, 1998-2004.	2.6	1
8	Methodological improvements for the analysis of domain movements in large biomolecular complexes. Biophysics and Physicobiology, 2019, 16, 328-336.	1.0	28
9	Morphing and docking visualisation of biomolecular structures using Multi-Dimensional Scaling. Journal of Molecular Graphics and Modelling, 2018, 82, 108-116.	2.4	6
10	Virtual Environment for Studying the Docking Interactions of Rigid Biomolecules with Haptics. Journal of Chemical Information and Modeling, 2017, 57, 1142-1152.	5.4	9
11	High quality rendering of protein dynamics in space filling mode. Journal of Molecular Graphics and Modelling, 2017, 78, 158-167.	2.4	4
12	Cover Image, Volume 85, Issue 10. Proteins: Structure, Function and Bioinformatics, 2017, 85, C1-C1.	2.6	1
13	Geometrical principles of homomeric Î²-barrels and Î²-helices: Application to modeling amyloid protofilaments. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1866-1881.	2.6	5
14	Determination of locked interfaces in biomolecular complexes using Haptimol_RD. Biophysics and Physicobiology, 2016, 13, 97-103.	1.0	5
15	The DynDom3D Webserver for the Analysis of Domain Movements in Multimeric Proteins. Journal of Computational Biology, 2016, 23, 21-26.	1.6	44
16	Monte Carlo Sampling with Linear Inverse Kinematics for Simulation of Protein Flexible Regions. Journal of Chemical Theory and Computation, 2015, 11, 3895-3905.	5.3	12
17	Adaptive GPU-accelerated force calculation for interactive rigid molecular docking using haptics. Journal of Molecular Graphics and Modelling, 2015, 61, 1-12.	2.4	11
18	Quantitative method for the assignment of hinge and shear mechanism in protein domain movements. Bioinformatics, 2014, 30, 3189-3196.	4.1	45

#	Article	IF	Citations
19	Rings and ribbons in protein structures: Characterization using helical parameters and Ramachandran plots for repeating dipeptides. Proteins: Structure, Function and Bioinformatics, 2014, 82, 230-239.	2.6	16
20	A real-time proximity querying algorithm for haptic-based molecular docking. Faraday Discussions, 2014, 169, 359-377.	3.2	10
21	Classification of Domain Movements in Proteins Using Dynamic Contact Graphs. PLoS ONE, 2013, 8, e81224.	2.5	18
22	Simulation of the Î²â€•to Î±â€sheet transition results in a twisted sheet for antiparallel and an Î±â€nanotube for parallel strands: Implications for amyloid formation. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3193-3207.	2.6	18
23	The Effect of End Constraints on Protein Loop Kinematics. Biophysical Journal, 2010, 98, 1976-1985.	0.5	5
24	DTA: dihedral transition analysis for characterization of the effects of large main-chain dihedral changes in proteins. Bioinformatics, 2009, 25, 628-635.	4.1	17
25	A method for the analysis of domain movements in large biomolecular complexes. Proteins: Structure, Function and Bioinformatics, 2009, 76, 201-212.	2.6	87
26	Interacting with the biomolecular solvent accessible surface via a haptic feedback device. BMC Structural Biology, 2009, 9, 69.	2.3	22
27	Database of ligand-induced domain movements in enzymes. BMC Structural Biology, 2009, 9, 13.	2.3	27
28	The geometry of Î±â€sheet: Implications for its possible function as amyloid precursor in proteins. Proteins: Structure, Function and Bioinformatics, 2008, 71, 415-425.	2.6	26
29	Peptide-plane flipping in proteins. Protein Science, 2008, 10, 2219-2227.	7.6	70
30	Essential dynamics sampling study of adenylate kinase: Comparison to citrate synthase and implication for the hinge and shear mechanisms of domain motions. Proteins: Structure, Function and Bioinformatics, 2007, 67, 325-337.	2.6	43
31	Molecular Dynamics Simulations of NAD+-Induced Domain Closure in Horse Liver Alcohol Dehydrogenase. Biophysical Journal, 2006, 91, 1823-1831.	0.5	34
32	Amyloid Formation May Involve Î±- to Î² Sheet Interconversion via Peptide Plane Flipping. Structure, 2006, 14, 1369-1376.	3.3	44
33	A comprehensive and non-redundant database of protein domain movements. Bioinformatics, 2005, 21, 2832-2838.	4.1	79
34	Investigating the Accessibility of the Closed Domain Conformation of Citrate Synthase using Essential Dynamics Sampling. Journal of Molecular Biology, 2004, 339, 515-525.	4.2	35
35	Identification of Specific Interactions that Drive Ligand-induced Closure in Five Enzymes with Classic Domain Movements. Journal of Molecular Biology, 2004, 339, 1001-1021.	4.2	75
36	The DynDom database of protein domain motions. Bioinformatics, 2003, 19, 1290-1291.	4.1	125

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37	Improvements in the analysis of domain motions in proteins from conformational change: DynDom version 1.50. Journal of Molecular Graphics and Modelling, 2002, 21, 181-183.	2.4	280
38	Investigation of the mechanism of domain closure in citrate synthase by molecular dynamics simulation 1 1Edited by R. Huber. Journal of Molecular Biology, 2001, 310, 1039-1053.	4.2	45
39	Structural principles governing domain motions in proteins. , 1999, 36, 425-435.		122
40	Structural principles governing domain motions in proteins. Proteins: Structure, Function and Bioinformatics, 1999, 36, 425-435.	2.6	3
41	Systematic analysis of domain motions in proteins from conformational change: New results on citrate synthase and T4 lysozyme. Proteins: Structure, Function and Bioinformatics, 1998, 30, 144-154.	2.6	746
42	Energy landscape of a native protein: Jumping-among-minima model. Proteins: Structure, Function and Bioinformatics, 1998, 33, 496-517.	2.6	242
43	Systematic analysis of domain motions in proteins from conformational change: New results on citrate synthase and T4 lysozyme. Proteins: Structure, Function and Bioinformatics, 1998, 30, 144-154.	2.6	8
44	Energy landscape of a native protein: Jumpingâ€amongâ€minima model. Proteins: Structure, Function and Bioinformatics, 1998, 33, 496-517.	2.6	4
45	Model-free methods of analyzing domain motions in proteins from simulation: A comparison of normal mode analysis and molecular dynamics simulation of lysozyme. , 1997, 27, 425-437.		241
46	Bending of the calmodulin central helix: A theoretical study. Protein Science, 1996, 5, 2044-2053.	7.6	71
47	Harmonicity and anharmonicity in protein dynamics: A normal mode analysis and principal component analysis. Proteins: Structure, Function and Bioinformatics, 1995, 23, 177-186.	2.6	140
48	Collective Variable Description of Native Protein Dynamics. Annual Review of Physical Chemistry, 1995, 46, 223-250.	10.8	249
49	Harmonic and anharmonic aspects in the dynamics of BPTI: A normal mode analysis and principal component analysis. Protein Science, 1994, 3, 936-943.	7.6	115
50	Comparison of normal mode analyses on a small globular protein in dihedral angle space and Cartesian coordinate space. Biophysical Chemistry, 1994, 52, 107-114.	2.8	32
51	Energy landscape of a native protein: Jumping-among-minima model. , 0, .		1
52	Energy landscape of a native protein: Jumping-among-minima model. , 0, .		1