Patrice Koehl

List of Publications by Year
in descending order

126 papers	7,021 citations	94381 37 h-index	62565 80 g-index
227 all docs	227 docs citations	227 times ranked	7346 citing authors

#	Article	IF	Citations
1	Plant NBS-LRR proteins: adaptable guards. Genome Biology, 2006, 7, 212.	13.9	804
2	The ASTRAL Compendium in 2004. Nucleic Acids Research, 2004, 32, 189D-192.	6.5	480
3	The ASTRAL compendium for protein structure and sequence analysis. Nucleic Acids Research, 2000, 28, 254-256.	6.5	432
4	Application of a Self-consistent Mean Field Theory to Predict Protein Side-chains Conformation and Estimate Their Conformational Entropy. Journal of Molecular Biology, 1994, 239, 249-275.	2.0	347
5	BAliBASE 3.0: Latest developments of the multiple sequence alignment benchmark. Proteins: Structure, Function and Bioinformatics, 2005, 61, 127-136.	1.5	343
6	NOMAD-Ref: visualization, deformation and refinement of macromolecular structures based on all-atom normal mode analysis. Nucleic Acids Research, 2006, 34, W52-W56.	6.5	292
7	Comprehensive Evaluation of Protein Structure Alignment Methods: Scoring by Geometric Measures. Journal of Molecular Biology, 2005, 346, 1173-1188.	2.0	260
8	Electrostatics calculations: latest methodological advances. Current Opinion in Structural Biology, 2006, 16, 142-151.	2.6	228
9	Small Libraries of Protein Fragments Model Native Protein Structures Accurately. Journal of Molecular Biology, 2002, 323, 297-307.	2.0	170
10	Single adduct mutagenesis: strong effect of the position of a single acetylaminofluorene adduct within a mutation hot spot.. Proceedings of the National Academy of Sciences of the United States of America, 1989, 86, 4147-4151.	3.3	163
11	Protein structure similarities. Current Opinion in Structural Biology, 2001, 11, 348-353.	2.6	158
12	Structural basis for ion permeation mechanism in pentameric ligand-gated ion channels. EMBO Journal, 2013, 32, 728-741.	3.5	140
13	Structure-based conformational preferences of amino acids. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 12524-12529.	3.3	129
14	De novo protein design. I. in search of stability and specificity 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1999, 293, 1161-1181.	2.0	122
15	ASTRAL compendium enhancements. Nucleic Acids Research, 2002, 30, 260-263.	6.5	117
16	Refined crystallographic structure of Pseudomonas aeruginosa exotoxin A and its implications for the molecular mechanism of toxicity 1 1Edited by D. Rees. Journal of Molecular Biology, 2001, 314, 823-837.	2.0	100
17	A self consistent mean field approach to simultaneous gap closure and side-chain positioning in homology modelling. Nature Structural and Molecular Biology, 1995, 2, 163-170.	3.6	97
18	Protein topology and stability define the space of allowed sequences. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 1280-1285.	3.3	94

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19	AquaSAXS: a web server for computation and fitting of SAXS profiles with non-uniformally hydrated atomic models. Nucleic Acids Research, 2011, 39, W184-W189.	6.5	91
20	Linear prediction spectral analysis of NMR data. Progress in Nuclear Magnetic Resonance Spectroscopy, 1999, 34, 257-299.	3.9	87
21	Polar and nonpolar atomic environments in the protein core: Implications for folding and binding. Proteins: Structure, Function and Bioinformatics, 1994, 20, 264-278.	1.5	86
22	Construction of plasmids containing a unique acetylaminofluorene adduct located within a mutation hot spot. Journal of Molecular Biology, 1989, 207, 355-364.	2.0	79
23	Mean-field minimization methods for biological macromolecules. Current Opinion in Structural Biology, 1996, 6, 222-226.	2.6	77
24	MinActionPath: maximum likelihood trajectory for large-scale structural transitions in a coarse-grained locally harmonic energy landscape. Nucleic Acids Research, 2007, 35, W477-W482.	6.5	76
25	De novo protein design. II. plasticity in sequence space 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1999, 293, 1183-1193.	2.0	74
26	Incorporating Dipolar Solvents with Variable Density in Poisson-Boltzmann Electrostatics. Biophysical Journal, 2008, 95, 5587-5605.	0.2	73
27	A New Lectin Family with Structure Similarity to Actinoporins Revealed by the Crystal Structure of Xerocomus chrysenteron Lectin XCL. Journal of Molecular Biology, 2004, 344, 1409-1420.	2.0	64
28	PDB_Hydro: incorporating dipolar solvents with variable density in the Poisson-Boltzmann treatment of macromolecule electrostatics. Nucleic Acids Research, 2006, 34, W38-W42.	6.5	62
29	Rod-derived Cone Viability Factor-2 is a novel bifunctional-thioredoxin-like protein with therapeutic potential. BMC Molecular Biology, 2007, 8, 74.	3.0	58
30	Sequence Variations within Protein Families are Linearly Related to Structural Variations. Journal of Molecular Biology, 2002, 323, 551-562.	2.0	57
31	Beyond the Poisson-Boltzmann Model: Modeling Biomolecule-Water and Water-Water Interactions. Physical Review Letters, 2009, 102, 087801.	2.9	56
32	Solution Structure of PMP-D2, a 35-Residue Peptide Isolated from the Insect Locusta migratoria. Biochemistry, 1994, 33, 15397-15407.	1.2	51
33	Algorithmic issues in modeling motion. ACM Computing Surveys, 2002, 34, 550-572.	16.1	51
34	The weighted-volume derivative of a space-filling diagram. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 2203-2208.	3.3	51
35	Strong structural effect of the position of a single acetylaminofluorene adduct within a mutation hot spot. Nucleic Acids Research, 1989, 17, 9531-9541.	6.5	48
36	<scp>AQUASOL</scp>: An efficient solver for the dipolar Poissonâ€“Boltzmannâ€“Langevin equation. Journal of Chemical Physics, 2010, 132, 064101.	1.2	44

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37	Accuracy of side-chain prediction upon near-native protein backbones generated by ab initio folding methods. , 1998, 33, 204-217.		42
38	Atomic Environment Energies in Proteins Defined from Statistics of Accessible and Contact Surface Areas. Journal of Molecular Biology, 1995, 249, 675-690.	2.0	36
39	Constructing side chains on near-native main chains for ab initio protein structure prediction. Protein Engineering, Design and Selection, 2000, 13, 453-457.	1.0	36
40	Computational Assembly of Polymorphic Amyloid Fibrils Reveals Stable Aggregates. Biophysical Journal, 2013, 104, 683-693.	0.2	36
41	Influence of protein structure databases on the predictive power of statistical pair potentials. , 1998, 31, 139-149.		34
42	Enhanced Amino Acid Selection in Fully Evolved Tryptophanyl-tRNA Synthetase, Relative to Its Urzyme, Requires Domain Motion Sensed by the D1 Switch, a Remote Dynamic Packing Motif. Journal of Biological Chemistry, 2014, 289, 4367-4376.	1.6	33
43	Structural Alphabets for Protein Structure Classification: A Comparison Study. Journal of Molecular Biology, 2009, 387, 431-450.	2.0	31
44	Landmark-free geometric methods in biological shape analysis. Journal of the Royal Society Interface, 2015, 12, 20150795.	1.5	31
45	Electrostatics, proton sensor, and networks governing the gating transition in GLIC, a proton-gated pentameric ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E12172-E12181.	3.3	30
46	Independent saturation of three TrpRS subsites generates a partially assembled state similar to those observed in molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 1790-1795.	3.3	28
47	Computing Ion Solvation Free Energies Using the Dipolar Poisson Model. Journal of Physical Chemistry B, 2009, 113, 5694-5697.	1.2	25
48	Helixâ€sheet packing in proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1736-1747.	1.5	25
49	Calculation of nuclear magnetic resonance order parameters in proteins by normal mode analysis. Journal of Chemical Physics, 1996, 104, 4768-4775.	1.2	24
50	Multi-Scale Clustering by Building a Robust and Self Correcting Ultrametric Topology on Data Points. PLoS ONE, 2013, 8, e56259.	1.1	24
51	MAO: a Multiple Alignment Ontology for nucleic acid and protein sequences. Nucleic Acids Research, 2005, 33, 4164-4171.	6.5	23
52	Geometric filtering of pairwise atomic interactions applied to the design of efficient statistical potentials. Computer Aided Geometric Design, 2006, 23, 531-544.	0.5	23
53	Ab initio sampling of transition paths by conditioned Langevin dynamics. Journal of Chemical Physics, 2017, 147, 152703.	1.2	22
54	Globally Optimal Cortical Surface Matching with Exact Landmark Correspondence. Lecture Notes in Computer Science, 2013, 23, 487-498.	1.0	22

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55	Solution Structure of Pyoverdin GM-II. Biochemistry, 1994, 33, 2843-2851.	1.2	21
56	The Area Derivative of a Space-Filling Diagram. Discrete and Computational Geometry, 2004, 32, 293.	0.4	21
57	Computing the geometry of a molecule in dihedral angle space using n.m.r.-derived constraints. Journal of Molecular Biology, 1992, 223, 299-315.	2.0	20
58	Selective and specific ion binding on proteins at physiologically-relevant concentrations. FEBS Letters, 2011, 585, 3126-3132.	1.3	20
59	Geometric measures of large biomolecules: Surface, volume, and pockets. Journal of Computational Chemistry, 2011, 32, 3023-3038.	1.5	20
60	Barbiturates Bind in the GLIC Ion Channel Pore and Cause Inhibition by Stabilizing a Closed State. Journal of Biological Chemistry, 2017, 292, 1550-1558.	1.6	19
61	1H nuclear magnetic resonance determination of the membrane-bound conformation of senktide, a highly selective neurokinin B agonist. Journal of Biomolecular NMR, 1993, 3, 443-61.	1.6	18
62	Improved recognition of native-like protein structures using a family of designed sequences. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 691-696.	3.3	18
63	The reconstruction of the relaxation matrix from an incomplete set of nuclear overhauser effects. Journal of Magnetic Resonance, 1990, 86, 565-583.	0.5	17
64	Fast Recursive Computation of 3D Geometric Moments from Surface Meshes. IEEE Transactions on Pattern Analysis and Machine Intelligence, 2012, 34, 2158-2163.	9.7	17
65	Identifying essential pairwise interactions in elastic network model using the alpha shape theory. Journal of Computational Chemistry, 2014, 35, 1111-1121.	1.5	17
66	3D representations of amino acidsâ€"applications to protein sequence comparison and classification. Computational and Structural Biotechnology Journal, 2014, 11, 47-58.	1.9	17
67	Visual Analysis of Biomolecular Surfaces. Mathematics and Visualization, 2008, , 237-255.	0.4	17
68	A quality metric for homology modeling: the H-factor. BMC Bioinformatics, 2011, 12, 48.	1.2	16
69	The Renormalization Group and Its Applications to Generating Coarse-Grained Models of Large Biological Molecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 1424-1438.	2.3	16
70	Surfaceâ€histogram: A new shape descriptor for proteinâ€protein docking. Proteins: Structure, Function and Bioinformatics, 2012, 80, 221-238.	1.5	15
71	Automatic Alignment of Genus-Zero Surfaces. IEEE Transactions on Pattern Analysis and Machine Intelligence, 2014, 36, 466-478.	9.7	15
72	Statistics and Limits of Linear-Prediction Quantification of Magnetic Resonance Spectral Parameters. Journal of Magnetic Resonance Series A, 1994, 109, 32-40.	1.6	14

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73	Building protein lattice models using self-consistent mean field theory. Journal of Chemical Physics, 1998, 108, 9540-9549.	1.2	14
74	Protein Structure Classification. Reviews in Computational Chemistry, 2006, , 1-55.	1.5	14
75	Large Eigenvalue Problems in Coarse-Grained Dynamic Analyses of Supramolecular Systems. Journal of Chemical Theory and Computation, 2018, 14, 3903-3919.	2.3	14
76	Modified Poissonâ€“Boltzmann equations for characterizing biomolecular solvation. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440001.	1.8	13
77	Protein side-chain modeling with a protein-dependent optimized rotamer library. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2000-2017.	1.5	13
78	Relaxed specificity in aromatic prenyltransferases. Nature Chemical Biology, 2005, 1, 71-72.	3.9	11
79	Comparative Normal Mode Analysis of the Dynamics of DENV and ZIKV Capsids. Frontiers in Molecular Biosciences, 2016, 3, 85.	1.6	11
80	Statistical Physics Approach to the Optimal Transport Problem. Physical Review Letters, 2019, 123, 040603.	2.9	11
81	Parameterizing elastic network models to capture the dynamics of proteins. Journal of Computational Chemistry, 2021, 42, 1643-1661.	1.5	11
82	Theory and simulation Can theory challenge experiment?. Current Opinion in Structural Biology, 1999, 9, 155-156.	2.6	10
83	Minimum action transition paths connecting minima on an energy surface. Journal of Chemical Physics, 2016, 145, 184111.	1.2	10
84	MEASURING THE SHAPES OF MACROMOLECULES â€“ AND WHY IT MATTERS. Computational and Structural Biotechnology Journal, 2013, 8, e201309001.	1.9	9
85	How round is a protein? Exploring protein structures for globularity using conformal mapping. Frontiers in Molecular Biosciences, 2014, 1, 26.	1.6	9
86	Bootstrapping on Undirected Binary Networks Via Statistical Mechanics. Journal of Statistical Physics, 2014, 156, 823-842.	0.5	9
87	Combined approaches from physics, statistics, and computer science for ab initio protein structure prediction: ex unitate vires (unity is strength)?. F1000Research, 2018, 7, 1125.	0.8	9
88	Adapting Poisson-Boltzmann to the self-consistent mean field theory: Application to protein side-chain modeling. Journal of Chemical Physics, 2011, 135, 055104.	1.2	8
89	An analytical method for computing atomic contact areas in biomolecules. Journal of Computational Chemistry, 2013, 34, 105-120.	1.5	8
90	Optimal transport at finite temperature. Physical Review E, 2019, 100, 013310.	0.8	8

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91	On the Importance of the Distance Measures Used to Train and Test Knowledge-Based Potentials for Proteins. PLoS ONE, 2014, 9, e109335.	1.1	8
92	Comparing shapes of genus-zero surfaces. Journal of Applied and Computational Topology, 2017, 1, 57-87.	1.0	7
93	Extracting information from RNA SHAPE data: Kalman filtering approach. PLoS ONE, 2018, 13, e0207029.	1.1	7
94	Structural and dynamic studies of two antigenic loops from haemagglutinin: A relaxation matrix approach. Journal of Biomolecular NMR, 1993, 3, 91-112.	1.6	6
95	The H-factor as a novel quality metric for homology modeling. Journal of Clinical Bioinformatics, 2012, 2, 18.	1.2	6
96	Capturing protein sequenceâ€“structure specificity using computational sequence design. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1556-1570.	1.5	6
97	His74 conservation in the bilin reductase PcyA family reflects an important role in protein-substrate structure and dynamics. Archives of Biochemistry and Biophysics, 2013, 537, 233-242.	1.4	6
98	Unraveling the Regional Specificities of Malbec Wines from Mendoza, Argentina, and from Northern California. Agronomy, 2019, 9, 234.	1.3	6
99	Physics approach to the variable-mass optimal-transport problem. Physical Review E, 2021, 103, 012113.	0.8	6
100	Morphing Methods to Visualize Coarse-Grained Protein Dynamics. Methods in Molecular Biology, 2014, 1084, 271-282.	0.4	5
101	Adaptive skin meshes coarsening for biomolecular simulation. Computer Aided Geometric Design, 2011, 28, 307-320.	0.5	4
102	Eleven quick tips for running an interdisciplinary short course for new graduate students. PLoS Computational Biology, 2018, 14, e1006039.	1.5	4
103	biDCG: A New Method for Discovering Global Features of DNA Microarray Data via an Iterative Re-Clustering Procedure. PLoS ONE, 2014, 9, e102445.	1.1	4
104	Fast measurement of heteronuclear relaxation: frequency-domain analysis of NMR accordion spectroscopy. Magnetic Resonance in Chemistry, 2001, 39, 447-456.	1.1	3
105	Extracting knowledge from protein structure geometry. Proteins: Structure, Function and Bioinformatics, 2013, 81, 841-851.	1.5	3
106	Unravelling the geometry of data matrices: effects of water stress regimes on winemaking. Journal of the Royal Society Interface, 2015, 12, 20150753.	1.5	3
107	String kernels for protein sequence comparisons: improved fold recognition. BMC Bioinformatics, 2017, 18, 137.	1.2	3
108	Coarse-grained dynamics of supramolecules: Conformational changes in outer shells of Dengue viruses. Progress in Biophysics and Molecular Biology, 2019, 143, 20-37.	1.4	3

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109	Sampling constrained stochastic trajectories using Brownian bridges. Journal of Chemical Physics, 2022, 157, .	1.2	3
110	A Geometric Representation of Protein Sequences. , 2007, , .		2
111	Sampling the conformation of protein surface residues for flexible protein docking. BMC Bioinformatics, 2010, 11, 575.	1.2	2
112	Mathematics's role in the grand challenge of deciphering the molecular basis of life. Frontiers in Molecular Biosciences, 2014, 1, 2.	1.6	2
113	Geometric Potentials for Computational Protein Sequence Design. Methods in Molecular Biology, 2017, 1529, 125-138.	0.4	2
114	DCG++: A data-driven metric for geometric pattern recognition. PLoS ONE, 2019, 14, e0217838.	1.1	2
115	Numerical Encodings of Amino Acids in Multivariate Gaussian Modeling of Protein Multiple Sequence Alignments. Molecules, 2019, 24, 104.	1.7	2
116	Fast computation of exact solutions of generic and degenerate assignment problems. Physical Review E, 2021, 103, 042101.	0.8	2
117	Molecular Force Fields. , 2009, , .		1
118	Protein Structure Prediction. , 2010, , 1-34.		1
119	PackHelix: A tool for helixâ€sheet packing during protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2828-2843.	1.5	1
120	Minimum action principle and shape dynamics. Journal of the Royal Society Interface, 2017, 14, 20170031.	1.5	1
121	A weighted string kernel for protein fold recognition. BMC Bioinformatics, 2017, 18, 378.	1.2	1
122	Simultaneous Identification of Multiple Binding Sites in Proteins: A Statistical Mechanics Approach. Journal of Physical Chemistry B, 2021, 125, 5052-5067.	1.2	1
123	Solvation of Ion Pairs: The Poisson-Langevin Model. , 2009, , .		0
124	Mortal Kombat: modeling amyloid fibrils and health implications. FASEB Journal, 2013, 27, 996.16.	0.2	0
125	Position of a Single Acetylaminofluorene Adduct Within a Mutational Hot Spot is Critical for the Related Mutagenic Event. , 1990, 52, 277-287.		0
126	Mutagenesis Induced by a Single Acetylaminofluorene Adduct Within the NarI Site is Position Dependent. , 1990, , 105-112.		0