Shalom Rackovsky

List of Publications by Year
in descending order

58	2,229	304743	214800
papers	citations	22 h-index	47 g-index

58	58	58	1340
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A united-residue force field for off-lattice protein-structure simulations. I. Functional forms and parameters of long-range side-chain interaction potentials from protein crystal data. Journal of Computational Chemistry, 1997, 18, 849-873.	3.3	334
2	New optimization method for conformational energy calculations on polypeptides: Conformational space annealing. Journal of Computational Chemistry, 1997, 18, 1222-1232.	3.3	291
3	A united-residue force field for off-lattice protein-structure simulations. II. Parameterization of short-range interactions and determination of weights of energy terms by Z-score optimization. Journal of Computational Chemistry, 1997, 18, 874-887.	3.3	183
4	United-residue force field for off-lattice protein-structure simulations: III. Origin of backbone hydrogen-bonding cooperativity in united-residue potentials. Journal of Computational Chemistry, 1998, 19, 259-276.	3.3	153
5	Prediction of protein conformation on the basis of a search for compact structures: Test on avian pancreatic polypeptide. Protein Science, 1993, 2, 1715-1731.	7.6	139
6	Calculation of protein backbone geometry from Î±â€carbon coordinates based on peptideâ€group dipole alignment. Protein Science, 1993, 2, 1697-1714.	7.6	98
7	Correlation of the structure of the transmembrane domain of the neu oncogene-encoded p185 protein with its function.. Proceedings of the National Academy of Sciences of the United States of America, 1990, 87, 8660-8664.	7.1	64
8	"Hidden" sequence periodicities and protein architecture. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 8580-8584.	7.1	64
9	Lessons from application of the UNRES force field to predictions of structures of CASP10 targets. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 14936-14941.	7.1	62
10	Quantitative organization of the known protein x-ray structures. I. Methods and short-length-scale results. Proteins: Structure, Function and Bioinformatics, 1990, 7, 378-402.	2.6	55
11	Hydrophobicity, hydrophilicity, and the radial and orientational distributions of residues in native proteins.. Proceedings of the National Academy of Sciences of the United States of America, 1977, 74, 5248-5251.	7.1	54
12	Intermolecular anti-parallel Â sheet: Comparison of predicted and observed conformations of gramicidin S. Proceedings of the National Academy of Sciences of the United States of America, 1980, 77, 6965-6967.	7.1	48
13	Effects of compact volume and chain stiffness on the conformations of native proteins.. Proceedings of the National Academy of Sciences of the United States of America, 1992, 89, 6614-6618.	7.1	42
14	Sequence physical properties encode the global organization of protein structure space. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 14345-14348.	7.1	42
15	On the nature of the protein folding code.. Proceedings of the National Academy of Sciences of the United States of America, 1993, 90, 644-648.	7.1	40
16	On the properties and sequence context of structurally ambivalent fragments in proteins. Protein Science, 2009, 12, 2420-2433.	7.6	36
17	Class-specific correlations between protein folding rate, structure-derived, and sequence-derived descriptors. Proteins: Structure, Function and Bioinformatics, 2003, 54, 333-341.	2.6	32
18	Improvement of the Treatment of Loop Structures in the UNRES Force Field by Inclusion of Coupling between Backbone- and Side-Chain-Local Conformational States. Journal of Chemical Theory and Computation, 2013, 9, 4620-4632.	5.3	30

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19	Comparative computational analysis of prion proteins reveals two fragments with unusual structural properties and a pattern of increase in hydrophobicity associated with disease-promoting mutations. Protein Science, 2009, 13, 3230-3244.	7.6	29
20	Optimally informative backbone structural propensities in proteins. Proteins: Structure, Function and Bioinformatics, 2002, 48, 463-486.	2.6	28
21	Optimized representations and maximal information in proteins. Proteins: Structure, Function and Bioinformatics, 2000, 38, 149-64.	2.6	28
22	Improvement of statistical potentials and threading score functions using information maximization. Proteins: Structure, Function and Bioinformatics, 2006, 62, 892-908.	2.6	26
23	Sequence-, structure-, and dynamics-based comparisons of structurally homologous CheY-like proteins. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 1578-1583.	7.1	24
24	Alternative approach to protein structure prediction based on sequential similarity of physical properties. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5029-5032.	7.1	23
25	Protein comparison and classification: a differential geometric approach.. Proceedings of the National Academy of Sciences of the United States of America, 1988, 85, 777-781.	7.1	22
26	Global characteristics of protein sequences and their implications. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 8623-8626.	7.1	22
27	Substitutions of proline 76 in yeast iso-1-cytochrome c. Analysis of residues compatible and incompatible with folding requirements. Journal of Biological Chemistry, 1985, 260, 13225-36.	3.4	21
28	On the redox conformational change in cytochrome c.. Proceedings of the National Academy of Sciences of the United States of America, 1984, 81, 5901-5905.	7.1	20
29	Homolog detection using global sequence properties suggests an alternate view of structural encoding in protein sequences. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5225-5229.	7.1	17
30	On the use of secondary structure in protein structure prediction: a bioinformatic analysis. Polymer, 2004, 45, 525-546.	3.8	16
31	Characterization of Architecture Signals in Proteinsâ€. Journal of Physical Chemistry B, 2006, 110, 18771-18778.	2.6	16
32	Information and discrimination in pairwise contact potentials. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1071-1087.	2.6	16
33	Spectral Analysis of a Protein Conformational Switch. Physical Review Letters, 2011, 106, 248101.	7.8	16
34	Protein sequence randomness and sequence/structure correlations. Biophysical Journal, 1995, 68, 1531-1539.	0.5	13
35	Nonlinearities in protein space limit the utility of informatics in protein biophysics. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1923-1928.	2.6	12
36	Prediction of conformation of rat galanin in the presence and absence of water with the use of monte Carlo methods and the ECEPP/3 force field. The Protein Journal, 1994, 13, 375-380.	1.1	11

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37	Discriminative ability with respect to amino acid types: Assessing the performance of knowledge-based potentials without threading. Proteins: Structure, Function and Bioinformatics, 2002, 49, 266-284.	2.6	11
38	Sequence determinants of protein architecture. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1681-1685.	2.6	10
39	The structure of protein dynamic space. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 19938-19942.	7.1	10
40	On the existence and implications of an inverse folding code in proteins.. Proceedings of the National Academy of Sciences of the United States of America, 1995, 92, 6861-6863.	7.1	9
41	Property-based sequence representations do not adequately encode local protein folding information. Proteins: Structure, Function and Bioinformatics, 2007, 67, 785-788.	2.6	9
42	On the Information Content of Protein Sequences. Journal of Biomolecular Structure and Dynamics, 2011, 28, 593-594.	3.5	9
43	Global informatics and physical property selection in protein sequences. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 1808-1810.	7.1	8
44	The structure of the carboxyl terminus of the p21 protein. Structural relationship to the nucleotide-binding/transforming regions of the protein. The Protein Journal, 1990, 9, 137-142.	1.1	6
45	Conformations of the central transforming region (Ile 55â€Met 67) of the p21 protein and their relationship to activation of the protein. International Journal of Peptide and Protein Research, 1990, 36, 247-254.	0.1	6
46	Sequenceâ€specific dynamic information in proteins. Proteins: Structure, Function and Bioinformatics, 2019, 87, 799-804.	2.6	6
47	Comparison of the predicted structure for the activated form of the P21 protein with the X-ray crystal structure. The Protein Journal, 1990, 9, 543-547.	1.1	4
48	Dynamic and conformational switching in proteins. Biopolymers, 2020, 112, e23411.	2.4	3
49	The dynamic basis of structural order in proteins. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1115-1118.	2.6	3
50	Computational analysis of variants of the operator binding domain of the bacteriophage ? repressor. International Journal of Quantum Chemistry, 1999, 75, 313-325.	2.0	2
51	A united-residue force field for off-lattice protein-structure simulations. I. Functional forms and parameters of long-range side-chain interaction potentials from protein crystal data. , 0, .		2
52	Identification of nonrandom patterns in structural and mutational data: the case of prion protein. , 0, , .		1
53	Beyond Supersecondary Structure: The Global Properties of Protein Sequences. Methods in Molecular Biology, 2012, 932, 107-114.	0.9	1
54	A united-residue force field for off-lattice protein-structure simulations. II. Parameterization of short-range interactions and determination of weights of energy terms by Z-score optimization. , 1997, 18, 874.		1

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55	CFP: a web-server for constructing sequence-based protein conformational flexibility profiles. Bioinformation, 2009, 4, 176-178.	0.5	1
56	Lattice Random Walk Theory of Geminate Recombination. Molecular Crystals and Liquid Crystals Incorporating Nonlinear Optics, 1989, 175, 135-140.	0.3	0
57	Beyond Supersecondary Structure: Physics-Based Sequence Alignment. Methods in Molecular Biology, 2019, 1958, 341-346.	0.9	0
58	Tribute to Harold A. Scheraga. Journal of Physical Chemistry B, 2020, 124, 10301-10302.	2.6	0