Stanislaw Oldziej

List of Publications by Citations

93 papers	2,975 citations	30 h-index	53 g-index
95 ext. papers	3,252 ext. citations	4.4 avg, IF	4.48 L-index

#	Paper	IF	Citations
93	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	3.5	286
92	Modification and optimization of the united-residue (UNRES) potential energy function for canonical simulations. I. Temperature dependence of the effective energy function and tests of the optimization method with single training proteins. *Journal of Physical Chemistry B*, **2007**, 111, 260-85	3.4	160
91	Recent improvements in prediction of protein structure by global optimization of a potential energy function. *Proceedings of the National Academy of Sciences of the United States of America*, **2001**, 98, 2329-33	11.5	144
90	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	3.5	142
89	Computational techniques for efficient conformational sampling of proteins. *Current Opinion in Structural Biology*, **2008**, 18, 134-9	8.1	137
88	Physics-based protein-structure prediction using a hierarchical protocol based on the UNRES force field: assessment in two blind tests. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 7547-52	11.5	120
87	A method for optimizing potential-energy functions by a hierarchical design of the potential-energy landscape: application to the UNRES force field. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 1937-42	11.5	111
86	Parametrization of Backbone Electrostatic and Multibody Contributions to the UNRES Force Field for Protein-Structure Prediction from Ab Initio Energy Surfaces of Model Systems *Journal of Physical Chemistry B*, **2004**, 108, 9421-9438	3.4	106
85	CAS MCSCF/CAS MCQDPT2 Study of the Mechanism of Singlet Oxygen Addition to 1,3-Butadiene and Benzene. *Journal of the American Chemical Society*, **2000**, 122, 8112-8119	16.4	85
84	A unified coarse-grained model of biological macromolecules based on mean-field multipole-multipole interactions. *Journal of Molecular Modeling*, **2014**, 20, 2306	2	83
83	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 3. Use of Many Proteins in Optimization. *Journal of Physical Chemistry B*, **2004**, 108, 16950-16959	3.4	70
82	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 2. Off-Lattice Tests of the Method with Single Proteins. *Journal of Physical Chemistry B*, **2004**, 108, 16934-16949	3.4	64
81	beta-hairpin-forming peptides; models of early stages of protein folding. *Biophysical Chemistry*, **2010**, 151, 1-9	3.5	59
80	Development of Physics-Based Energy Functions that Predict Medium-Resolution Structures for Proteins of the and Structural Classes. *Journal of Physical Chemistry B*, **2001**, 105, 7299-7311	3.4	59
79	Mean-field interactions between nucleic-acid-base dipoles can drive the formation of a double helix. *Physical Review Letters*, **2013**, 110, 098101	7.4	58
78	Determination of the Potentials of Mean Force for Rotation about C Virtual Bonds in Polypeptides from the ab Initio Energy Surfaces of Terminally Blocked Glycine, Alanine, and Proline *Journal of Physical Chemistry A*, **2003**, 107, 8035-8046	2.8	58
77	Simulation of the opening and closing of Hsp70 chaperones by coarse-grained molecular dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 1750-1764	6.4	54

76	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, 14936-41	11.5	54
75	Potential of mean force of hydrophobic association: dependence on solute size. *Journal of Physical Chemistry B*, **2007**, 111, 10765-74	3.4	54
74	Exploration of the conformational space of oxytocin and arginine-vasopressin using the electrostatically driven Monte Carlo and molecular dynamics methods. *Biopolymers*, **1996**, 38, 157-75	2.2	51
73	Conformational dynamics of the trp-cage miniprotein at its folding temperature. *Journal of Physical Chemistry B*, **2012**, 116, 6898-907	3.4	46
72	Azapeptides structurally based upon inhibitory sites of cystatins as potent and selective inhibitors of cysteine proteases. *Journal of Medicinal Chemistry*, **2002**, 45, 4202-11	8.3	39
71	Implementation of molecular dynamics and its extensions with the coarse-grained UNRES force field on massively parallel systems; towards millisecond-scale simulations of protein structure, dynamics, and thermodynamics. *Journal of Chemical Theory and Computation*, **2010**, 6, 890-909	6.4	37
70	Dynamic Formation and Breaking of Disulfide Bonds in Molecular Dynamics Simulations with the UNRES Force Field. *Journal of Chemical Theory and Computation*, **2007**, 3, 1236-48	6.4	36
69	Disulfide bonding arrangements in active forms of the somatomedin B domain of human vitronectin. *Biochemistry*, **2004**, 43, 6519-34	3.2	35
68	Simple physics-based analytical formulas for the potentials of mean force for the interaction of amino acid side chains in water. IV. Pairs of different hydrophobic side chains. *Journal of Physical Chemistry B*, **2008**, 112, 11385-95	3.4	34
67	Maximum Likelihood Calibration of the UNRES Force Field for Simulation of Protein Structure and Dynamics. *Journal of Chemical Information and Modeling*, **2017**, 57, 2364-2377	6.1	33
66	The copper(II) coordination abilities of three novel cyclic tetrapeptides with -His-Xaa-His- motif. *Journal of Inorganic Biochemistry*, **2007**, 101, 452-60	4.2	33
65	Simple physics-based analytical formulas for the potentials of mean force for the interaction of amino acid side chains in water. 3. Calculation and parameterization of the potentials of mean force of pairs of identical hydrophobic side chains. *Journal of Physical Chemistry B*, **2007**, 111, 2925-31	3.4	30
64	Improved conformational space annealing method to treat ╫structure with the UNRES force-field and to enhance scalability of parallel implementation. *Polymer*, **2004**, 45, 677-686	3.9	30
63	Maximum entropy approach to the determination of solution conformation of flexible polypeptides by global conformational analysis and NMR spectroscopy--application to DNS1-c-[D-A2,bu2,Trp4,Leu5]enkephalin and DNS1-c-[D-A2bu2,Trp4,D-Leu5]enkephalin. *Journal of*	3	30
62	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,	6.4	29
61	Evidence, from simulations, of a single state with residual native structure at the thermal denaturation midpoint of a small globular protein. *Journal of the American Chemical Society*, **2010**, 132, 9444-52	16.4	29
60	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 1. Tests of the Approach Using Simple Lattice Protein Models. *Journal of Physical Chemistry B*, **2004**, 108, 16918-16933	3.4	29
59	A Maximum-Likelihood Approach to Force-Field Calibration. *Journal of Chemical Information and Modeling*, **2015**, 55, 2050-70	6.1	27

58	Prediction of the structures of proteins with the UNRES force field, including dynamic formation and breaking of disulfide bonds. *Protein Engineering, Design and Selection*, **2004**, 17, 29-36	1.9	27
57	Impact of ring size on the copper(II) coordination abilities of cyclic tetrapeptides. *Journal of Inorganic Biochemistry*, **2009**, 103, 813-7	4.2	25
56	Protein structure prediction with the UNRES force-field using Replica-Exchange Monte Carlo-with-Minimization; Comparison with MCM, CSA, and CFMC. *Journal of Computational Chemistry*, **2005**, 26, 1472-86	3.5	25
55	A general method for the derivation of the functional forms of the effective energy terms in coarse-grained energy functions of polymers. III. Determination of scale-consistent backbone-local and correlation potentials in the UNRES force field and force-field calibration and validation. *Journal of Chemical Physics*, **2012**, 150, 155104	3.9	24
54	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. I. Importance of hydrophobic interactions in stabilization of beta-hairpin structure. *Proteins: Structure, Function and Bioinformatics*, **2009**, 75, 931-53	4.2	22
53	Prediction of protein structure using a knowledge-based off-lattice united-residue force field and global optimization methods. *Theoretical Chemistry Accounts*, **1999**, 101, 16-20	1.9	21
52	Qualitative and Quantitative Analysis of Proteome and Peptidome of Human Follicular Fluid Using Multiple Samples from Single Donor with LC-MS and SWATH Methodology. *Journal of Proteome Research*, **2017**, 16, 3053-3067	5.6	20
51	Towards temperature-dependent coarse-grained potentials of side-chain interactions for protein folding simulations. I: molecular dynamics study of a pair of methane molecules in water at various temperatures. *Protein Engineering, Design and Selection*, **2009**, 22, 547-52	1.9	20
50	A united residue force-field for calcium-protein interactions. *Protein Science*, **2004**, 13, 2725-35	6.3	18
49	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. II. Interplay of local backbone conformational dynamics and long-range hydrophobic interactions in hairpin formation. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 637-54	4.2	17
48	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. *Scientific Reports*, **2018**, 8, 9939	4.9	16
47	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin-binding protein G from Streptococcus. IV. Implication for the mechanism of folding of the parent protein. *Biopolymers*, **2010**, 93, 469-80	2.2	16
46	Chelating ability and biological activity of hesperetin Schiff base. *Journal of Inorganic Biochemistry*, **2015**, 143, 34-47	4.2	14
45	The influence of the cyclopeptide sequence on its coordination abilities towards Cu(II). *Polyhedron*, **2010**, 29, 1535-1542	2.7	14
44	Conformational studies of the C-terminal 16-amino-acid-residue fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. *Biopolymers*, **2009**, 91, 37-51	2.2	12
43	Impact of 1,5-disubstituted tetrazole ring on chelating ability of delta-selective opioid peptide. *Journal of Inorganic Biochemistry*, **2004**, 98, 447-58	4.2	11
42	Human follicular fluid proteomic and peptidomic composition quantitative studies by SWATH-MS methodology. Applicability of high pH RP-HPLC fractionation. *Journal of Proteomics*, **2019**, 191, 131-142	3.9	11
41	The unusual stabilization of the Ni2+ and Cu2+ complexes with NSFRY. *Dalton Transactions*, **2013**, 42, 448-58	4.3	10

40	Conformational studies of the alpha-helical 28-43 fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. *Biopolymers*, **2008**, 89, 1032-44	2.2	10
39	Unusual gain in the coordination ability of vasopressin-like peptides towards Cu2+ ions by insertion of the highly hydrophobic side chain. *New Journal of Chemistry*, **2003**, 27, 251-256	3.6	10
38	Impact of Cu(II) and Ni(II) on a structure of chiral peptide nucleic acids having four, six and eight thymines in a peptide side chain. *Journal of Inorganic Biochemistry*, **2001**, 85, 79-87	4.2	10
37	Chiral peptide nucleic acids having thymine and adenine in their side chain as specific ligands for NiII and CuII. *Dalton Transactions RSC*, **2000**, 2639-2644		10
36	Coarse-Grained Models of Proteins: Theory and Applications **2011**, 35-83		10
35	Use of NMR and fluorescence spectroscopy as well as theoretical conformational analysis in conformation-activity studies of cyclic enkephalin analogues. *Current Topics in Medicinal Chemistry*, **2004**, 4, 123-33	3	9
34	Coordination ability of pentapeptides with two dehydro-amino acid residues inserted into their sequences. *Journal of Inorganic Biochemistry*, **2004**, 98, 1391-8	4.2	9
33	Molecular modeling of the catalytic domain of serine/threonine phosphatase-1 with the Zn2+ and Mn2+ di-nuclear ion centers in the active site. *Computers & Chemistry*, **2000**, 24, 381-90		9
32	The photophysics of ╫homo-tyrosine and its simple derivatives. *Journal of Photochemistry and Photobiology A: Chemistry*, **1996**, 101, 171-181	4.7	9
31	Mechanism of formation of the C-terminal beta-hairpin of the B3 domain of the immunoglobulin binding protein G from Streptococcus. III. Dynamics of long-range hydrophobic interactions. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 723-37	4.2	8
30	The Photophysics of ╫Tyrosine and Its Simple Derivatives. *Journal of Fluorescence*, **1997**, 7, 257-266	2.4	8
29	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, 375-80		8
28	Unique and Universal Features of Epsilonproteobacterial Origins of Chromosome Replication and DnaA-DnaA Box Interactions. *Frontiers in Microbiology*, **2016**, 7, 1555	5.7	8
27	Toward temperature-dependent coarse-grained potentials of side-chain interactions for protein folding simulations. II. Molecular dynamics study of pairs of different types of interactions in water at various temperatures. *Journal of Physical Chemistry B*, **2012**, 116, 6844-53	3.4	7
26	Fluorescence and Monte Carlo conformational studies of the (1-15) galanin amide fragment. *Biophysical Chemistry*, **1996**, 58, 303-12	3.5	7
25	Combination of SAXS and NMR Techniques as a Tool for the Determination of Peptide Structure in Solution. *Journal of Physical Chemistry Letters*, **2010**, 1, 3128-3131	6.4	6
24	Conformational aspects of differences in requirements for oxytocin and vasopressin receptors. *Journal of Receptor and Signal Transduction Research*, **1995**, 15, 703-13	2.6	6
23	Coordination ability of insect kinin analogs. *Polyhedron*, **2009**, 28, 485-492	2.7	5

22	Fluorescence study of neurohypophyseal hormones and their analogues. Distance distributions in a series of arginine-vasopressin analogues. *European Biophysics Journal*, **1997**, 26, 183-93	1.9	5
21	A new approach to the resolution of the excitation-emission spectra of multicomponent systems. *Computers & Chemistry*, **1997**, 21, 89-96		5
20	MNDO study of the mechanism of the inhibition of cysteine proteinases by diazomethyl ketones. *European Biophysics Journal*, **1992**, 21, 217-22	1.9	5
19	Theoretical Studies of Interactions between O-Phosphorylated and Standard Amino-Acid Side-Chain Models in Water. *Journal of Physical Chemistry B*, **2015**, 119, 8526-34	3.4	4
18	Gain-of-function mutation in complement C2 protein identified in a patient with aHUS. *Journal of Allergy and Clinical Immunology*, **2020**, 146, 916-919.e11	11.5	4
17	A Hierarchical Multiscale Approach to Protein Structure Prediction: Production of Low-Resolution Packing Arrangements of Helices and Refinement of the Best Models with a United-Residue Force Field. *Multiscale Modeling and Simulation*, **2006**, 5, 1175-1195	1.8	4
16	Towards Temperature Dependent Coarse-grained Potential of Side-chain Interactions for Protein Folding Simulations **2010**,		3
15	Impact of histidine residue on chelating ability of 2Sdeoxyriboadenosine. *Journal of Inorganic Biochemistry*, **2011**, 105, 1212-9	4.2	3
14	Mechanism of action of aspartic proteinases: application of transition-state analogue theory. *Journal of Computer-Aided Molecular Design*, **1996**, 10, 583-8	4.2	3
13	Effect of tetrazole moiety on coordinating efficiency of deltorphin.. *Acta Biochimica Polonica*, **2004**, 51, 93-106	2	3
12	Ab initio study of the mechanism of singlet-dioxygen addition to hydroxyaromatic compounds: negative evidence for the involvement of peroxa and endoperoxide intermediates. *Journal of Computational Chemistry*, **2002**, 23, 1076-89	3.5	2
11	Photophysical properties of homo-tyrosine derivatives. *Amino Acids*, **1996**, 10, 197-200	3.5	2
10	Investigation of the inhibition pathway of glucosamine synthase by N3-(4-methoxyfumaroyl)-L-2,3-diaminopropanoic acid by semiempirical quantum mechanical and molecular mechanics methods. *European Biophysics Journal*, **1992**, 21, 273-80	1.9	2
9	Meta-computations on the CLUSTERIX Grid **2007**, 489-500		2
8	AfsK-Mediated Site-Specific Phosphorylation Regulates DnaA Initiator Protein Activity in Streptomyces coelicolor. *Journal of Bacteriology*, **2020**, 202,	3.5	1
7	1.21 Computation of Structure, Dynamics, and Thermodynamics of Proteins **2012**, 494-513		1
6	Microscopic Physics-Based Models of Proteins and Nucleic Acids **2017**, 67-120		1
5	Compatibility of Distinct Label-Free Proteomic Workflows in Absolute Quantification of Proteins Linked to the Oocyte Quality in Human Follicular Fluid. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1

List of Publications

4	Gain-of-Function Mutations R249C and S250C in Complement C2 Protein Increase C3 Deposition in the Presence of C-Reactive Protein.. *Frontiers in Immunology*, **2021**, 12, 724361	8.4	0
3	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. *Methods in Molecular Biology*, **2022**, 2376, 399-416	1.4	0
2	Chemoinformatics Methods for Studying Biomolecules **2017**, 2183-2199		
1	Chemoinformatics Methods for Studying Biomolecules **2016**, 1-17		