

Stanislaw Oldziej

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Modeling the Structure, Dynamics, and Transformations of Proteins with the UNRES Force Field. <i>Methods in Molecular Biology</i> , 2022 , 2376, 399-416	1.4	0
92	Gain-of-Function Mutations R249C and S250C in Complement C2 Protein Increase C3 Deposition in the Presence of C-Reactive Protein.. <i>Frontiers in Immunology</i> , 2021 , 12, 724361	8.4	0
91	Compatibility of Distinct Label-Free Proteomic Workflows in Absolute Quantification of Proteins Linked to the Oocyte Quality in Human Follicular Fluid. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	1
90	AfsK-Mediated Site-Specific Phosphorylation Regulates DnaA Initiator Protein Activity in <i>Streptomyces coelicolor</i> . <i>Journal of Bacteriology</i> , 2020 , 202,	3.5	1
89	Gain-of-function mutation in complement C2 protein identified in a patient with aHUS. <i>Journal of Allergy and Clinical Immunology</i> , 2020 , 146, 916-919.e11	11.5	4
88	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. <i>Journal of Chemical Physics</i> , 2019 , 150, 155104	3.9	24
87	Human follicular fluid proteomic and peptidomic composition quantitative studies by SWATH-MS methodology. Applicability of high pH RP-HPLC fractionation. <i>Journal of Proteomics</i> , 2019 , 191, 131-142	3.9	11
86	An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12. <i>Scientific Reports</i> , 2018 , 8, 9939	4.9	16
85	Chemoinformatics Methods for Studying Biomolecules 2017 , 2183-2199		
84	Maximum Likelihood Calibration of the UNRES Force Field for Simulation of Protein Structure and Dynamics. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 2364-2377	6.1	33
83	Qualitative and Quantitative Analysis of Proteome and Peptidome of Human Follicular Fluid Using Multiple Samples from Single Donor with LC-MS and SWATH Methodology. <i>Journal of Proteome Research</i> , 2017 , 16, 3053-3067	5.6	20
82	Microscopic Physics-Based Models of Proteins and Nucleic Acids 2017 , 67-120		1
81	Chemoinformatics Methods for Studying Biomolecules 2016 , 1-17		
80	Unique and Universal Features of Epsilonproteobacterial Origins of Chromosome Replication and DnaA-DnaA Box Interactions. <i>Frontiers in Microbiology</i> , 2016 , 7, 1555	5.7	8
79	Theoretical Studies of Interactions between O-Phosphorylated and Standard Amino-Acid Side-Chain Models in Water. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 8526-34	3.4	4
78	A Maximum-Likelihood Approach to Force-Field Calibration. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2050-70	6.1	27
77	Chelating ability and biological activity of hesperetin Schiff base. <i>Journal of Inorganic Biochemistry</i> , 2015 , 143, 34-47	4.2	14

76	A unified coarse-grained model of biological macromolecules based on mean-field multipole-multipole interactions. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2306	2	83
75	Improvement of the treatment of loop structures in the UNRES force field by inclusion of coupling between backbone- and side-chain-local conformational states. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9,	6.4	29
74	The unusual stabilization of the Ni ²⁺ and Cu ²⁺ complexes with NSF _{RY} . <i>Dalton Transactions</i> , 2013 , 42, 448-58	4.3	10
73	Mean-field interactions between nucleic-acid-base dipoles can drive the formation of a double helix. <i>Physical Review Letters</i> , 2013 , 110, 098101	7.4	58
72	Lessons from application of the UNRES force field to predictions of structures of CASP10 targets. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 14936-41	11.5	54
71	Simulation of the opening and closing of Hsp70 chaperones by coarse-grained molecular dynamics. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 1750-1764	6.4	54
70	Conformational dynamics of the trp-cage miniprotein at its folding temperature. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6898-907	3.4	46
69	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. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 6844-53	3.4	7
68	1.21 Computation of Structure, Dynamics, and Thermodynamics of Proteins 2012 , 494-513		1
67	Impact of histidine residue on chelating ability of 2Sdeoxyriboadenosine. <i>Journal of Inorganic Biochemistry</i> , 2011 , 105, 1212-9	4.2	3
66	Coarse-Grained Models of Proteins: Theory and Applications 2011 , 35-83		10
65	Towards Temperature Dependent Coarse-grained Potential of Side-chain Interactions for Protein Folding Simulations 2010 ,		3
64	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. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 890-909	6.4	37
63	Evidence, from simulations, of a single state with residual native structure at the thermal denaturation midpoint of a small globular protein. <i>Journal of the American Chemical Society</i> , 2010 , 132, 9444-52	16.4	29
62	Combination of SAXS and NMR Techniques as a Tool for the Determination of Peptide Structure in Solution. <i>Journal of Physical Chemistry Letters</i> , 2010 , 1, 3128-3131	6.4	6
61	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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 723-37	4.2	8
60	beta-hairpin-forming peptides; models of early stages of protein folding. <i>Biophysical Chemistry</i> , 2010 , 151, 1-9	3.5	59
59	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. <i>Biopolymers</i> , 2010 , 93, 469-80	2.2	16

58	The influence of the cyclopeptide sequence on its coordination abilities towards Cu(II). <i>Polyhedron</i> , 2010 , 29, 1535-1542	2.7	14
57	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. <i>Protein Engineering, Design and Selection</i> , 2009 , 22, 547-52	1.9	20
56	Conformational studies of the C-terminal 16-amino-acid-residue fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. <i>Biopolymers</i> , 2009 , 91, 37-51	2.2	12
55	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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 75, 931-53	4.2	22
54	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. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009 , 76, 637-54	4.2	17
53	Impact of ring size on the copper(II) coordination abilities of cyclic tetrapeptides. <i>Journal of Inorganic Biochemistry</i> , 2009 , 103, 813-7	4.2	25
52	Coordination ability of insect kinin analogs. <i>Polyhedron</i> , 2009 , 28, 485-492	2.7	5
51	Computational techniques for efficient conformational sampling of proteins. <i>Current Opinion in Structural Biology</i> , 2008 , 18, 134-9	8.1	137
50	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. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 11385-95	3.4	34
49	Conformational studies of the alpha-helical 28-43 fragment of the B3 domain of the immunoglobulin binding protein G from Streptococcus. <i>Biopolymers</i> , 2008 , 89, 1032-44	2.2	10
48	Dynamic Formation and Breaking of Disulfide Bonds in Molecular Dynamics Simulations with the UNRES Force Field. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1236-48	6.4	36
47	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. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 2925-31	3.4	30
46	Potential of mean force of hydrophobic association: dependence on solute size. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 10765-74	3.4	54
45	The copper(II) coordination abilities of three novel cyclic tetrapeptides with -His-Xaa-His- motif. <i>Journal of Inorganic Biochemistry</i> , 2007 , 101, 452-60	4.2	33
44	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. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 260-85	3.4	160
43	Meta-computations on the CLUSTERIX Grid 2007 , 489-500		2
42	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. <i>Multiscale Modeling and Simulation</i> , 2006 , 5, 1175-1195	1.8	4
41	Protein structure prediction with the UNRES force-field using Replica-Exchange Monte Carlo-with-Minimization; Comparison with MCM, CSA, and CFMC. <i>Journal of Computational Chemistry</i> , 2005 , 26, 1472-86	3.5	25

40	Physics-based protein-structure prediction using a hierarchical protocol based on the UNRES force field: assessment in two blind tests. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005 , 102, 7547-52	11.5	120
39	A united residue force-field for calcium-protein interactions. <i>Protein Science</i> , 2004 , 13, 2725-35	6.3	18
38	Use of NMR and fluorescence spectroscopy as well as theoretical conformational analysis in conformation-activity studies of cyclic enkephalin analogues. <i>Current Topics in Medicinal Chemistry</i> , 2004 , 4, 123-33	3	9
37	Prediction of the structures of proteins with the UNRES force field, including dynamic formation and breaking of disulfide bonds. <i>Protein Engineering, Design and Selection</i> , 2004 , 17, 29-36	1.9	27
36	Impact of 1,5-disubstituted tetrazole ring on chelating ability of delta-selective opioid peptide. <i>Journal of Inorganic Biochemistry</i> , 2004 , 98, 447-58	4.2	11
35	Coordination ability of pentapeptides with two dehydro-amino acid residues inserted into their sequences. <i>Journal of Inorganic Biochemistry</i> , 2004 , 98, 1391-8	4.2	9
34	Improved conformational space annealing method to treat structure with the UNRES force-field and to enhance scalability of parallel implementation. <i>Polymer</i> , 2004 , 45, 677-686	3.9	30
33	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 2. Off-Lattice Tests of the Method with Single Proteins. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 16934-16949	3.4	64
32	Parametrization of Backbone Electrostatic and Multibody Contributions to the UNRES Force Field for Protein-Structure Prediction from Ab Initio Energy Surfaces of Model Systems. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 9421-9438	3.4	106
31	Disulfide bonding arrangements in active forms of the somatomedin B domain of human vitronectin. <i>Biochemistry</i> , 2004 , 43, 6519-34	3.2	35
30	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 3. Use of Many Proteins in Optimization. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 16950-16959	3.4	70
29	Optimization of the UNRES Force Field by Hierarchical Design of the Potential-Energy Landscape. 1. Tests of the Approach Using Simple Lattice Protein Models. <i>Journal of Physical Chemistry B</i> , 2004 , 108, 16918-16933	3.4	29
28	Effect of tetrazole moiety on coordinating efficiency of deltorphin.. <i>Acta Biochimica Polonica</i> , 2004 , 51, 93-106	2	3
27	Determination of the Potentials of Mean Force for Rotation about C-C Virtual Bonds in Polypeptides from the ab Initio Energy Surfaces of Terminally Blocked Glycine, Alanine, and Proline. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 8035-8046	2.8	58
26	Unusual gain in the coordination ability of vasopressin-like peptides towards Cu ²⁺ ions by insertion of the highly hydrophobic side chain. <i>New Journal of Chemistry</i> , 2003 , 27, 251-256	3.6	10
25	Ab initio study of the mechanism of singlet-dioxygen addition to hydroxyaromatic compounds: negative evidence for the involvement of peroxa and endoperoxide intermediates. <i>Journal of Computational Chemistry</i> , 2002 , 23, 1076-89	3.5	2
24	A method for optimizing potential-energy functions by a hierarchical design of the potential-energy landscape: application to the UNRES force field. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 1937-42	11.5	111
23	Azapeptides structurally based upon inhibitory sites of cystatins as potent and selective inhibitors of cysteine proteases. <i>Journal of Medicinal Chemistry</i> , 2002 , 45, 4202-11	8.3	39

22	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. <i>Journal of Inorganic Biochemistry</i> , 2001 , 85, 79-87	4.2	10
21	Recent improvements in prediction of protein structure by global optimization of a potential energy function. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2001 , 98, 2329-33	11.5	144
20	Development of Physics-Based Energy Functions that Predict Medium-Resolution Structures for Proteins of the α and β Structural Classes. <i>Journal of Physical Chemistry B</i> , 2001 , 105, 7299-7311	3.4	59
19	Molecular modeling of the catalytic domain of serine/threonine phosphatase-1 with the Zn ²⁺ and Mn ²⁺ di-nuclear ion centers in the active site. <i>Computers & Chemistry</i> , 2000 , 24, 381-90		9
18	Chiral peptide nucleic acids having thymine and adenine in their side chain as specific ligands for Ni(II) and Cu(II). <i>Dalton Transactions RSC</i> , 2000 , 2639-2644		10
17	CAS MCSCF/CAS MCQDPT2 Study of the Mechanism of Singlet Oxygen Addition to 1,3-Butadiene and Benzene. <i>Journal of the American Chemical Society</i> , 2000 , 122, 8112-8119	16.4	85
16	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-A2 bu2, Trp4, D-Leu5]enkephalin. <i>Journal of Biomolecular NMR</i> , 1999 , 15, 315-30	3	30
15	Prediction of protein structure using a knowledge-based off-lattice united-residue force field and global optimization methods. <i>Theoretical Chemistry Accounts</i> , 1999 , 101, 16-20	1.9	21
14	United-residue force field for off-lattice protein-structure simulations: III. Origin of backbone hydrogen-bonding cooperativity in united-residue potentials. <i>Journal of Computational Chemistry</i> , 1998 , 19, 259-276	3.5	142
13	The Photophysics of β -Tyrosine and Its Simple Derivatives. <i>Journal of Fluorescence</i> , 1997 , 7, 257-266	2.4	8
12	Fluorescence study of neurohypophyseal hormones and their analogues. Distance distributions in a series of arginine-vasopressin analogues. <i>European Biophysics Journal</i> , 1997 , 26, 183-93	1.9	5
11	A new approach to the resolution of the excitation-emission spectra of multicomponent systems. <i>Computers & Chemistry</i> , 1997 , 21, 89-96		5
10	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. <i>Journal of Computational Chemistry</i> , 1997 , 18, 849-873	3.5	286
9	Exploration of the conformational space of oxytocin and arginine-vasopressin using the electrostatically driven Monte Carlo and molecular dynamics methods. <i>Biopolymers</i> , 1996 , 38, 157-75	2.2	51
8	Fluorescence and Monte Carlo conformational studies of the (1-15) galanin amide fragment. <i>Biophysical Chemistry</i> , 1996 , 58, 303-12	3.5	7
7	The photophysics of β -tyrosine and its simple derivatives. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 1996 , 101, 171-181	4.7	9
6	Photophysical properties of β -tyrosine derivatives. <i>Amino Acids</i> , 1996 , 10, 197-200	3.5	2
5	Mechanism of action of aspartic proteinases: application of transition-state analogue theory. <i>Journal of Computer-Aided Molecular Design</i> , 1996 , 10, 583-8	4.2	3

4	Conformational aspects of differences in requirements for oxytocin and vasopressin receptors. <i>Journal of Receptor and Signal Transduction Research</i> , 1995 , 15, 703-13	2.6	6
3	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. <i>The Protein Journal</i> , 1994 , 13, 375-80		8
2	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. <i>European Biophysics Journal</i> , 1992 , 21, 273-80	1.9	2
1	MNDO study of the mechanism of the inhibition of cysteine proteinases by diazomethyl ketones. <i>European Biophysics Journal</i> , 1992 , 21, 217-22	1.9	5