Martin Zacharias

List of Publications by Year
in descending order

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230 papers	8,131 citations	44069 48 h-index	71685 76 g-index

247 all docs	247 docs citations	247 times ranked	8338 citing authors

#	Article	IF	Citations
1	Match_Motif: A rapid computational tool to assist in proteinâ€“protein interaction design. Protein Science, 2022, 31, 147-157.	7.6	1
2	Altered fibrin clot structure and dysregulated fibrinolysis contribute toÂthrombosis risk in severe COVID-19. Blood Advances, 2022, 6, 1074-1087.	5.2	35
3	Molecular rationale for the impairment of the MexAB-OprM efflux pump by a single mutation in MexA. Computational and Structural Biotechnology Journal, 2022, 20, 252-260.	4.1	4
4	Computational Tools for Accurate Binding Free-Energy Prediction. Methods in Molecular Biology, 2022, 2385, 255-292.	0.9	3
5	Cryo-EM demonstrates the in vitro proliferation of an ex vivo amyloid fibril morphology by seeding. Nature Communications, 2022, 13, 85.	12.8	15
6	Rapid Rational Design of Cyclic Peptides Mimicking Proteinâ€“Protein Interfaces. Methods in Molecular Biology, 2022, 2405, 231-244.	0.9	1
7	Dissociation of Î²2m from MHC class I triggers formation of noncovalent transient heavy chain dimers. Journal of Cell Science, 2022, 135, .	2.0	6
8	The Impact of Prolonged Inflammation on Wound Healing. Biomedicines, 2022, 10, 856.	3.2	33
9	Nearest-Neighbor dsDNA Stability Analysis Using Alchemical Free-Energy Simulations. Journal of Physical Chemistry B, 2022, , .	2.6	1
10	Active site geometry stabilization of a presenilin homolog by the lipid bilayer promotes intramembrane proteolysis. ELife, 2022, 11, .	6.0	3
11	An internal docking site stabilizes substrate binding to Î³-secretase: Analysis by molecular dynamics simulations. Biophysical Journal, 2022, 121, 2330-2344.	0.5	10
12	ADAMTS4-specific MR probe to assess aortic aneurysms in vivo using synthetic peptide libraries. Nature Communications, 2022, 13, .	12.8	6
13	Improving the Potential of Mean Force and Nonequilibrium Pulling Simulations by Simultaneous Alchemical Modifications. Journal of Chemical Theory and Computation, 2022, 18, 3873-3893.	5.3	5
14	Analysis of amyloidogenic transthyretin mutations using continuum solvent free energy calculations. Proteins: Structure, Function and Bioinformatics, 2022, 90, 2080-2090.	2.6	2
15	Explicit solvent repulsive scaling replica exchange molecular dynamics (<scp>RSâ€REMD</scp>) in molecular modeling of proteinâ€glycosaminoglycan complexes. Journal of Computational Chemistry, 2022, 43, 1633-1640.	3.3	6
16	Targeting Telomeres: Molecular Dynamics and Free Energy Simulation of Gold-Carbene Binding to DNA. Biophysical Journal, 2021, 120, 101-108.	0.5	3
17	Proteolysis of Rab32 by Salmonella GtgE induces an inactive GTPase conformation. IScience, 2021, 24, 101940.	4.1	12
18	Evaluation of replica exchange with repulsive scaling approach for docking glycosaminoglycans. Journal of Computational Chemistry, 2021, 42, 1040-1053.	3.3	8

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19	Specificity of AMPylation of the human chaperone BiP is mediated by TPR motifs of FICD. Nature Communications, 2021, 12, 2426.	12.8	15
20	Accurate modeling of DNA conformational flexibility by a multivariate Ising model. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	35
21	Controlling Protein Crystallization by Free Energy Guided Design of Interactions at Crystal Contacts. Crystals, 2021, 11, 588.	2.2	4
22	Between inflammation and thrombosis: endothelial cells in COVID-19. European Respiratory Journal, 2021, 58, 2100377.	6.7	86
23	Rapid Antigen Test for Postmortem Evaluation of SARS-CoV-2 Carriage. Emerging Infectious Diseases, 2021, 27, 1734-1737.	4.3	14
24	Influence of a Ser111â€phosphorylation on Rab1b GTPase conformational dynamics studied by advanced sampling simulations. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1324-1332.	2.6	0
25	Molecular and Spectroscopic Characterization of Green and Red Cyanine Fluorophores from the Alexa Fluor and AF Series**. ChemPhysChem, 2021, 22, 1566-1583.	2.1	27
26	Mechanism of collagen folding propagation studied by Molecular Dynamics simulations. PLoS Computational Biology, 2021, 17, e1009079.	3.2	9
27	Molecular and Spectroscopic Characterization of Green and Red Cyanine Fluorophores from the Alexa Fluor and AF Series. ChemPhysChem, 2021, 22, 1546-1546.	2.1	8
28	Molecular insights on CALX-CBD12 interdomain dynamics from MD simulations, RDCs, and SAXS. Biophysical Journal, 2021, 120, 3664-3675.	0.5	4
29	Modeling Proteinâ€“Glycosaminoglycan Complexes: Does the Size Matter?. Journal of Chemical Information and Modeling, 2021, 61, 4475-4485.	5.4	14
30	Molecular mechanism of amyloidogenic mutations in hypervariable regions of antibody light chains. Journal of Biological Chemistry, 2021, 296, 100334.	3.4	22
31	Tumuc1: A New Accurate DNA Force Field Consistent with High-Level Quantum Chemistry. Journal of Chemical Theory and Computation, 2021, 17, 7096-7105.	5.3	21
32	Structural dynamics in the evolution of a bilobed protein scaffold. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	9
33	Binding-induced functional-domain motions in the Argonaute characterized by adaptive advanced sampling. PLoS Computational Biology, 2021, 17, e1009625.	3.2	6
34	Reflex testing in non-small cell lung carcinoma using DNA- and RNA-based next-generation sequencingâ€”a single-center experience. Translational Lung Cancer Research, 2021, 10, 4221-4234.	2.8	7
35	Orientation Dependence of DNA Blunt-End Stacking Studied by Free-Energy Simulations. Journal of Physical Chemistry B, 2021, 125, 13850-13857.	2.6	4
36	Computational prediction of proteinâ€“protein binding affinities. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1448.	14.6	107

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37	Molecular mechanism of Be²⁺-ion binding to HLA-DP2: tetrahedral coordination, conformational changes and multi-ion binding. Physical Chemistry Chemical Physics, 2020, 22, 799-810.	2.8	8
38	How Mutations Perturb Î³-Secretase Active Site Studied by Free Energy Simulations. ACS Chemical Neuroscience, 2020, 11, 3321-3332.	3.5	14
39	Occurrence of SARS-CoV-2 in the intraocular milieu. Experimental Eye Research, 2020, 201, 108273.	2.6	18
40	From monomer to fibril: Abetaâ€amyloid binding to Aducanumab antibody studied by molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1592-1606.	2.6	12
41	Ligand binding and global adaptation of the GlnPQ substrate binding domain 2 revealed by molecular dynamics simulations. Protein Science, 2020, 29, 2482-2494.	7.6	5
42	Altered Hinge Conformations in APP Transmembrane Helix Mutants May Affect Enzymeâ€“Substrate Interactions of Î³-Secretase. ACS Chemical Neuroscience, 2020, 11, 4426-4433.	3.5	12
43	CHARMM-GUI supports the Amber force fields. Journal of Chemical Physics, 2020, 153, 035103.	3.0	175
44	Efficient Refinement and Free Energy Scoring of Predicted Proteinâ€“Protein Complexes Using Replica Exchange with Repulsive Scaling. Journal of Chemical Information and Modeling, 2020, 60, 5552-5562.	5.4	20
45	Rapid in silico Design of Potential Cyclic Peptide Binders Targeting Protein-Protein Interfaces. Frontiers in Chemistry, 2020, 8, 573259.	3.6	16
46	Base-Pairing and Base-Stacking Contributions to Double-Stranded DNA Formation. Journal of Physical Chemistry B, 2020, 124, 10345-10352.	2.6	20
47	Folding and Unfolding of the Short Light-Triggered Î²-Hairpin Peptide AzoChignolin Occurs within 100 ns. Journal of Physical Chemistry B, 2020, 124, 5113-5121.	2.6	3
48	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
49	How global DNA unwinding causes non-uniform stress distribution and melting of DNA. PLoS ONE, 2020, 15, e0232976.	2.5	19
50	Prediction of proteinâ€“protein complexes using replica exchange with repulsive scaling. Journal of Computational Chemistry, 2020, 41, 1436-1447.	3.3	27
51	Structures of peptide-free and partially loaded MHC class I molecules reveal mechanisms of peptide selection. Nature Communications, 2020, 11, 1314.	12.8	40
52	Compensatory Mechanisms in Temperature Dependence of DNA Double Helical Structure: Bending and Elongation. Journal of Chemical Theory and Computation, 2020, 16, 2857-2863.	5.3	16
53	Coarseâ€grained and atomic resolution biomolecular docking with the ATTRACT approach. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1018-1028.	2.6	12
54	The dynamics of Î³-secretase and its substrates. Seminars in Cell and Developmental Biology, 2020, 105, 86-101.	5.0	19

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55	Fatal amyloid formation in a patientâ€™s antibody light chain is caused by a single point mutation. ELife, 2020, 9, .	6.0	33
56	Prediction of proteinâ€“protein complex structures by docking. , 2020, , 59-85.		0
57	How global DNA unwinding causes non-uniform stress distribution and melting of DNA. , 2020, 15, e0232976.		0
58	How global DNA unwinding causes non-uniform stress distribution and melting of DNA. , 2020, 15, e0232976.		0
59	How global DNA unwinding causes non-uniform stress distribution and melting of DNA. , 2020, 15, e0232976.		0
60	How global DNA unwinding causes non-uniform stress distribution and melting of DNA. , 2020, 15, e0232976.		0
61	Phosphorylation of Ser111 in Rab8a Modulates Rabin8-Dependent Activation by Perturbation of Side Chain Interaction Networks. Biochemistry, 2019, 58, 3546-3554.	2.5	8
62	Empty peptide-receptive MHC class I molecules for efficient detection of antigen-specific T cells. Science Immunology, 2019, 4, .	11.9	64
63	Cryo-EM structure of a transthyretin-derived amyloid fibril from a patient with hereditary ATTR amyloidosis. Nature Communications, 2019, 10, 5008.	12.8	127
64	The Architecture of Talin1 Reveals an Autoinhibition Mechanism. Cell, 2019, 179, 120-131.e13.	28.9	93
65	Evaluation of Predicted Proteinâ€“Protein Complexes by Binding Free Energy Simulations. Journal of Chemical Theory and Computation, 2019, 15, 2071-2086.	5.3	46
66	Prognostic value of cyclin A2 and B1 expression in lung carcinoids. Pathology, 2019, 51, 481-486.	0.6	20
67	Uncovering the Binding Mode of Î³ -Secretase Inhibitors. ACS Chemical Neuroscience, 2019, 10, 3398-3403.	3.5	21
68	Extracellular interface between APP and Nicastrin regulates AÎ² length and response to Î³â€secretase modulators. EMBO Journal, 2019, 38, .	7.8	45
69	An Interspecies Analysis Reveals Molecular Construction Principles of Interleukin 27. Journal of Molecular Biology, 2019, 431, 2383-2393.	4.2	10
70	Dynamics of the full-length yeast Hsp90 dimer. European Physical Journal: Special Topics, 2019, 227, 1693-1704.	2.6	1
71	Free energy calculations elucidate substrate binding, gating mechanism, and toleranceâ€promoting mutations in herbicide target 4â€hydroxyphenylpyruvate dioxygenase. Protein Science, 2019, 28, 1048-1058.	7.6	9
72	How methylâ€“sugar interactions determine DNA structure and flexibility. Nucleic Acids Research, 2019, 47, 1132-1140.	14.5	21

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73	Atomic Resolution Insight into Sac7d Protein Binding to DNA and Associated Global Changes by Molecular Dynamics Simulations. Angewandte Chemie - International Edition, 2019, 58, 5967-5972.	13.8	8
74	Modeling large proteinâ€“glycosaminoglycan complexes using a fragmentâ€based approach. Journal of Computational Chemistry, 2019, 40, 1429-1439.	3.3	15
75	Atomic Resolution Insight into Sac7d Protein Binding to DNA and Associated Global Changes by Molecular Dynamics Simulations. Angewandte Chemie, 2019, 131, 6028-6033.	2.0	1
76	Global Dynamics of Yeast Hsp90 Middle and C-Terminal Dimer Studied by Advanced Sampling Simulations. Frontiers in Molecular Biosciences, 2019, 6, 93.	3.5	4
77	The structure and oxidation of the eye lens chaperone Î±A-crystallin. Nature Structural and Molecular Biology, 2019, 26, 1141-1150.	8.2	42
78	A folding switch regulates interleukin 27 biogenesis and secretion of its Î±-subunit as a cytokine. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1585-1590.	7.1	32
79	Structural Modeling of Î³-Secretase AÎ²_n Complex Formation and Substrate Processing. ACS Chemical Neuroscience, 2019, 10, 1826-1840.	3.5	25
80	The N-Terminal Segment of the Voltage-Dependent Anion Channel: A Possible Membrane-Bound Intermediate in Pore Unbinding. Journal of Molecular Biology, 2019, 431, 223-243.	4.2	10
81	Structural Architecture of the Nucleosome Remodeler ISWI Determined from Cross-Linking, Mass Spectrometry, SAXS, and Modeling. Structure, 2018, 26, 282-294.e6.	3.3	11
82	A single residue switch reveals principles of antibody domain integrity. Journal of Biological Chemistry, 2018, 293, 17107-17118.	3.4	8
83	Bulk tumour cell migration in lung carcinomas might be more common than epithelial-mesenchymal transition and be differently regulated. BMC Cancer, 2018, 18, 717.	2.6	33
84	Tethered multifluorophore motion reveals equilibrium transition kinetics of single DNA double helices. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7512-E7521.	7.1	33
85	The temperature dependence of the helical twist of DNA. Nucleic Acids Research, 2018, 46, 7998-8009.	14.5	55
86	Î³-Secretase Studied by Atomistic Molecular Dynamics Simulations: Global Dynamics, Enzyme Activation, Water Distribution and Lipid Binding. Frontiers in Chemistry, 2018, 6, 640.	3.6	29
87	Both DNA global deformation and repair enzyme contacts mediate flipping of thymine dimer damage. Scientific Reports, 2017, 7, 41324.	3.3	13
88	Predicting Allosteric Changes from Conformational Ensembles. Structure, 2017, 25, 393-394.	3.3	3
89	Monte Carlo replica-exchange based ensemble docking of protein conformations. Proteins: Structure, Function and Bioinformatics, 2017, 85, 924-937.	2.6	15
90	Optical control of a receptor-linked guanylyl cyclase using a photoswitchable peptidic hormone. Chemical Science, 2017, 8, 4644-4653.	7.4	23

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91	Thermodynamics and Kinetics of Nucleobase Stacking Oligomerization Revealed by Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 3005-3011.	5.3	4
92	Fast and accurate grid representations for atomâ€based docking with partner flexibility. Journal of Computational Chemistry, 2017, 38, 1538-1546.	3.3	1
93	Multidomain structure and correlated dynamics determined by self-consistent FRET networks. Nature Methods, 2017, 14, 174-180.	19.0	110
94	The pepATTRACT web server for blind, large-scale peptideâ€“protein docking. Nucleic Acids Research, 2017, 45, W361-W364.	14.5	84
95	Origin of Ion Specificity of Telomeric DNA G-Quadruplexes Investigated by Free-Energy Simulations. Biophysical Journal, 2017, 112, 2280-2290.	0.5	18
96	From Aβ2 Filament to Fibril: Molecular Mechanism of Surface-Activated Secondary Nucleation from All-Atom MD Simulations. Journal of Physical Chemistry B, 2017, 121, 671-682.	2.6	34
97	Determinants of the assembly and function of antibody variable domains. Scientific Reports, 2017, 7, 12276.	3.3	20
98	Comparative Molecular Dynamics Analysis of RNase-S Complex Formation. Biophysical Journal, 2017, 113, 1466-1474.	0.5	8
99	Multiscale Simulation of Receptorâ€“Drug Association Kinetics: Application to Neuraminidase Inhibitors. Journal of Chemical Theory and Computation, 2017, 13, 5097-5105.	5.3	24
100	Unwinding Induced Melting of Double-Stranded DNA Studied by Free Energy Simulations. Journal of Physical Chemistry B, 2017, 121, 11019-11030.	2.6	27
101	Proteinâ€protein and peptideâ€protein docking and refinement using ATTRACT in CAPRI. Proteins: Structure, Function and Bioinformatics, 2017, 85, 391-398.	2.6	18
102	Update of the ATTRACT force field for the prediction of protein-protein binding affinity. Journal of Computational Chemistry, 2017, 38, 1887-1890.	3.3	9
103	Rapid Design of Knowledge-Based Scoring Potentials for Enrichment of Near-Native Geometries in Protein-Protein Docking. PLoS ONE, 2017, 12, e0170625.	2.5	7
104	Accelerated flexible protein-ligand docking using Hamiltonian replica exchange with a repulsive biasing potential. PLoS ONE, 2017, 12, e0172072.	2.5	14
105	Transient helicity in intrinsically disordered Axin-1 studied by NMR spectroscopy and molecular dynamics simulations. PLoS ONE, 2017, 12, e0174337.	2.5	7
106	Covalent dye attachment influences the dynamics and conformational properties of flexible peptides. PLoS ONE, 2017, 12, e0177139.	2.5	18
107	Concerted regulation of ISWI by an autoinhibitory domain and the H4 N-terminal tail. ELife, 2017, 6, .	6.0	28
108	Application of the ATTRACT Coarse-Grained Docking and Atomistic Refinement for Predicting Peptide-Protein Interactions. Methods in Molecular Biology, 2017, 1561, 49-68.	0.9	0

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109	Rapid approximate calculation of water binding free energies in the whole hydration domain of (bio)macromolecules. Journal of Computational Chemistry, 2016, 37, 1711-1724.	3.3	2
110	Adenylylation of Tyr77 stabilizes Rab1b GTPase in an active state: A molecular dynamics simulation analysis. Scientific Reports, 2016, 6, 19896.	3.3	13
111	Regulatory Implications of Non-Trivial Splicing: Isoform 3 of Rab1A Shows Enhanced Basal Activity and Is Not Controlled by Accessory Proteins. Journal of Molecular Biology, 2016, 428, 1544-1557.	4.2	5
112	Single-molecule dissection of stacking forces in DNA. Science, 2016, 353, .	12.6	180
113	Free energy analysis and mechanism of base pair stacking in nicked DNA. Nucleic Acids Research, 2016, 44, gkw607.	14.5	60
114	Global deformation facilitates flipping of damaged 8-oxo-guanine and guanine in DNA. Nucleic Acids Research, 2016, 44, gkw827.	14.5	12
115	Structure and target interaction of a G-quadruplex RNA-aptamer. RNA Biology, 2016, 13, 973-987.	3.1	20
116	SAXS Data Alone can Generate High-Quality Models of Protein-Protein Complexes. Structure, 2016, 24, 1387-1397.	3.3	40
117	Fragment-based modelling of single stranded RNA bound to RNA recognition motif containing proteins. Nucleic Acids Research, 2016, 44, 4565-4580.	14.5	20
118	Cryo-EM Data Are Superior to Contact and Interface Information in Integrative Modeling. Biophysical Journal, 2016, 110, 785-797.	0.5	14
119	A Stable Mutant Predisposes Antibody Domains to Amyloid Formation through Specific Non-Native Interactions. Journal of Molecular Biology, 2016, 428, 1315-1332.	4.2	20
120	Dynamics of Seeded AÎ²₄₀-Fibril Growth from Atomistic Molecular Dynamics Simulations: Kinetic Trapping and Reduced Water Mobility in the Locking Step. Journal of the American Chemical Society, 2016, 138, 527-539.	13.7	77
121	Binding Site Identification and Flexible Docking of Single Stranded RNA to Proteins Using a Fragment-Based Approach. PLoS Computational Biology, 2016, 12, e1004697.	3.2	19
122	Development and Application of a Fully Blind Flexible Peptide-protein Docking Protocol, pepATTRACT. Bio-protocol, 2016, 6, .	0.4	0
123	Free Energy Calculations of Ligandâ€“Protein Binding. , 2015, , 313-335.		1
124	Explaining the striking difference in twist-stretch coupling between DNA and RNA: A comparative molecular dynamics analysis. Nucleic Acids Research, 2015, 43, gkv1028.	14.5	50
125	Application of Enhanced Sampling Monte Carlo Methods for High-Resolution Protein-Protein Docking in Rosetta. PLoS ONE, 2015, 10, e0125941.	2.5	24
126	A Compact Native 24-Residue Supersecondary Structure Derived from the Villin Headpiece Subdomain. Biophysical Journal, 2015, 108, 678-686.	0.5	7

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127	Effect O6â€guanine alkylation on DNA flexibility studied by comparative molecular dynamics simulations. Biopolymers, 2015, 103, 23-32.	2.4	3
128	A Web Interface for Easy Flexible Protein-Protein Docking with ATTRACT. Biophysical Journal, 2015, 108, 462-465.	0.5	82
129	Exploring biomolecular dynamics and interactions using advanced sampling methods. Journal of Physics Condensed Matter, 2015, 27, 323101.	1.8	27
130	Fully Blind Peptide-Protein Docking with pepATTRACT. Structure, 2015, 23, 1507-1515.	3.3	112
131	Influence of a cis,synâ€cyclobutane pyrimidine dimer damage on DNA conformation studied by molecular dynamics simulations. Biopolymers, 2015, 103, 215-222.	2.4	7
132	The Antibody Light-Chain Linker Is Important for Domain Stability and Amyloid Formation. Journal of Molecular Biology, 2015, 427, 3572-3586.	4.2	21
133	RAID3 - An interleukin-6 receptor-binding aptamer with post-selective modification-resistant affinity. RNA Biology, 2015, 12, 1043-1053.	3.1	23
134	Substrate Binding Specifically Modulates Domain Arrangements in Adenylate Kinase. Biophysical Journal, 2015, 109, 1978-1985.	0.5	17
135	iATTRACT: Simultaneous global and local interface optimization for proteinâ€“protein docking refinement. Proteins: Structure, Function and Bioinformatics, 2015, 83, 248-258.	2.6	57
136	Rapid Alchemical Free Energy Calculation Employing a Generalized Born Implicit Solvent Model. Journal of Physical Chemistry B, 2015, 119, 968-975.	2.6	7
137	Coupling between side chain interactions and binding pocket flexibility in HLA-B*44:02 molecules investigated by molecular dynamics simulations. Molecular Immunology, 2015, 63, 312-319.	2.2	18
138	An Integrative Approach to the Study of Filamentous Oligomeric Assemblies, with Application to RecA. PLoS ONE, 2015, 10, e0116414.	2.5	14
139	Computational Antigenic Epitope Prediction by Calculating Electrostatic Desolvation Penalties of Protein Surfaces. Methods in Molecular Biology, 2014, 1184, 365-374.	0.9	2
140	PEP-SiteFinder: a tool for the blind identification of peptide binding sites on protein surfaces. Nucleic Acids Research, 2014, 42, W221-W226.	14.5	79
141	A Residue-specific Shift in Stability and Amyloidogenicity of Antibody Variable Domains. Journal of Biological Chemistry, 2014, 289, 26829-26846.	3.4	15
142	Efficient calculation of relative binding free energies by umbrella sampling perturbation. Journal of Computational Chemistry, 2014, 35, 2256-2262.	3.3	18
143	Hamiltonian replicaâ€exchange simulations with adaptive biasing of peptide backbone and side chain dihedral angles. Journal of Computational Chemistry, 2014, 35, 150-158.	3.3	28
144	Stabilization of duplex DNA and RNA by dangling ends studied by free energy simulations. Biopolymers, 2014, 101, 418-427.	2.4	13

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145	Theoretical studies of nucleic acids folding. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 116-126.	14.6	4
146	Enhanced conformational sampling of carbohydrates by Hamiltonian replica-exchange simulation. Glycobiology, 2014, 24, 70-84.	2.5	24
147	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	2.6	50
148	Evaluation of Generalized Born Model Accuracy for Absolute Binding Free Energy Calculations. Journal of Physical Chemistry B, 2014, 118, 7467-7474.	2.6	18
149	Proteinâ€“Ligand Docking Using Hamiltonian Replica Exchange Simulations with Soft Core Potentials. Journal of Chemical Information and Modeling, 2014, 54, 1669-1675.	5.4	32
150	Adaptive Biasing Combined with Hamiltonian Replica Exchange to Improve Umbrella Sampling Free Energy Simulations. Journal of Chemical Theory and Computation, 2014, 10, 703-710.	5.3	23
151	Hamiltonian replica exchange combined with elastic network analysis to enhance global domain motions in atomistic molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3410-3419.	2.6	10
152	Role of Tryptophan Side Chain Dynamics on the Trp-Cage Mini-Protein Folding Studied by Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e88383.	2.5	26
153	Flexible docking and refinement with a coarseâ€grained protein model using ATTRACT. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2167-2174.	2.6	57
154	Role of tyrosine hotâ€spot residues at the interface of colicin E9 and immunity protein 9: A comparative free energy simulation study. Proteins: Structure, Function and Bioinformatics, 2013, 81, 461-468.	2.6	10
155	Redirecting catalysis from proteolysis to perhydrolysis in subtilisin Carlsberg. Journal of Biotechnology, 2013, 167, 279-286.	3.8	6
156	Influence of 8-Oxoguanosine on the Fine Structure of DNA Studied with Biasing-Potential Replica Exchange Simulations. Biophysical Journal, 2013, 104, 1089-1097.	0.5	20
157	Advanced replica-exchange sampling to study the flexibility and plasticity of peptides and proteins. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 847-853.	2.3	62
158	Elastic Network Models of Nucleic Acids Flexibility. Journal of Chemical Theory and Computation, 2013, 9, 5460-5470.	5.3	29
159	Effect of 8-Oxoguanine on DNA Structure and Deformability. Journal of Physical Chemistry B, 2013, 117, 11617-11622.	2.6	17
160	Combining coarseâ€grained nonbonded and atomistic bonded interactions for protein modeling. Proteins: Structure, Function and Bioinformatics, 2013, 81, 81-92.	2.6	24
161	gp130 activation is regulated by D2â€“D3 interdomain connectivity. Biochemical Journal, 2013, 450, 487-496.	3.7	20
162	Dipeptides promote folding and peptide binding of MHC class I molecules. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 15383-15388.	7.1	55

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163	Reengineering of subtilisin Carlsberg for oxidative resistance. Biological Chemistry, 2013, 394, 79-87.	2.5	8
164	Combining geometric pocket detection and desolvation properties to detect putative ligand binding sites on proteins. Journal of Structural Biology, 2012, 180, 546-550.	2.8	14
165	Protein-DNA docking with a coarse-grained force field. BMC Bioinformatics, 2012, 13, 228.	2.6	31
166	ATTRACT and PTOOLS: Open Source Programs for Proteinâ€“Protein Docking. Methods in Molecular Biology, 2012, 819, 221-232.	0.9	18
167	Atomic resolution model of the antibody Fc interaction with the complement C1q component. Molecular Immunology, 2012, 51, 66-72.	2.2	34
168	Scoring optimisation of unbound proteinâ€“protein docking including protein binding site predictions. Journal of Molecular Recognition, 2012, 25, 15-23.	2.1	10
169	ReFlexIn: A Flexible Receptor Protein-Ligand Docking Scheme Evaluated on HIV-1 Protease. PLoS ONE, 2012, 7, e48008.	2.5	10
170	ATTRACT-EM: A New Method for the Computational Assembly of Large Molecular Machines Using Cryo-EM Maps. PLoS ONE, 2012, 7, e49733.	2.5	45
171	Role of the closing base pair for d(GCA) hairpin stability: free energy analysis and folding simulations. Nucleic Acids Research, 2011, 39, 8271-8280.	14.5	13
172	Application of biasing-potential replica exchange simulations for loop modeling and refinement of proteins in explicit solvent. Journal of Cheminformatics, 2011, 3, .	6.1	1
173	Efficient inclusion of receptor flexibility in gridâ€based proteinâ€“ligand docking*. Journal of Computational Chemistry, 2011, 32, 3433-3439.	3.3	27
174	A coarse-grained force field for Proteinâ€“RNA docking. Nucleic Acids Research, 2011, 39, 9118-9129.	14.5	55
175	Tapasin dependence of major histocompatibility complex class I molecules correlates with their conformational flexibility. FASEB Journal, 2011, 25, 3989-3998.	0.5	61
176	Rationalizing perhydrolase activity of aryl-esterase and subtilisin Carlsberg mutants by molecular dynamics simulations of the second tetrahedral intermediate state. Theoretical Chemistry Accounts, 2010, 125, 375-386.	1.4	9
177	Accounting for conformational changes during proteinâ€“protein docking. Current Opinion in Structural Biology, 2010, 20, 180-186.	5.7	141
178	Adv. Eng. Mater. 1-2/2010. Advanced Engineering Materials, 2010, 12, NA-NA.	3.5	0
179	Bovine Serum Albumin and Lysozyme Adsorption on Calcium Phosphate Particles. Advanced Engineering Materials, 2010, 12, B53.	3.5	31
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