

Emil Alexov

List of Publications by Year in descending order

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136
papers

7,436
citations

53660

45
h-index

62479

80
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140
all docs

140
docs citations

140
times ranked

7923
citing authors

#	ARTICLE	IF	CITATIONS
1	Protein-Protein Binding Free Energy Predictions with the MM/PBSA Approach Complemented with the Gaussian-Based Method for Entropy Estimation. <i>ACS Omega</i> , 2022, 7, 11057-11067.	1.6	9
2	A regularization approach for solving the super-Gaussian Poisson-Boltzmann model with heterogeneous dielectric functions. <i>Journal of Computational Physics</i> , 2022, 464, 111340.	1.9	4
3	SAAMBE-SEQ: a sequence-based method for predicting mutation effect on protein-protein binding affinity. <i>Bioinformatics</i> , 2021, 37, 992-999.	1.8	17
4	SAAFEC-SEQ: A Sequence-Based Method for Predicting the Effect of Single Point Mutations on Protein Thermodynamic Stability. <i>International Journal of Molecular Sciences</i> , 2021, 22, 606.	1.8	63
5	On regularization of charge singularities in solving the Poisson-Boltzmann equation with a smooth solute-solvent boundary. <i>Mathematical Biosciences and Engineering</i> , 2021, 18, 1370-1405.	1.0	6
6	Increased p53 signaling impairs neural differentiation in HUWE1-promoted intellectual disabilities. <i>Cell Reports Medicine</i> , 2021, 2, 100240.	3.3	5
7	Computational Investigation of the pH Dependence of Stability of Melanosome Proteins: Implication for Melanosome formation and Disease. <i>International Journal of Molecular Sciences</i> , 2021, 22, 8273.	1.8	2
8	SAMPDI-3D: predicting the effects of protein and DNA mutations on protein-DNA interactions. <i>Bioinformatics</i> , 2021, 37, 3760-3765.	1.8	8
9	Opioid Addiction and Opioid Receptor Dimerization: Structural Modeling of the OPRD1 and OPRM1 Heterodimer and Its Signaling Pathways. <i>International Journal of Molecular Sciences</i> , 2021, 22, 10290.	1.8	3
10	pH-Dependent Interactions of Apolipoprotein III with a Lipid Disk. <i>Journal of Computational Biophysics and Chemistry</i> , 2021, 20, 153-164.	1.0	4
11	BION-2: Predicting Positions of Non-Specifically Bound Ions on Protein Surface by a Gaussian-Based Treatment of Electrostatics. <i>International Journal of Molecular Sciences</i> , 2021, 22, 272.	1.8	5
12	Computational chemistry methods to investigate the effects caused by DNA variants linked with disease. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 1930001.	1.8	2
13	An Ensemble Approach to Predict the Pathogenicity of Synonymous Variants. <i>Genes</i> , 2020, 11, 1102.	1.0	6
14	Ab-initio binding of barnase-barstar with DelPhiForce steered Molecular Dynamics (DFMD) approach. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2050016.	1.8	2
15	Mutations in FAM50A suggest that Armfield XLID syndrome is a spliceosomopathy. <i>Nature Communications</i> , 2020, 11, 3698.	5.8	38
16	Capturing the Effects of Explicit Waters in Implicit Electrostatics Modeling: Qualitative Justification of Gaussian-Based Dielectric Models in DelPhi. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2229-2246.	2.5	8
17	In-silico analysis to identify the role of MEN1 missense mutations in breast cancer. <i>Journal of Theoretical and Computational Chemistry</i> , 2020, 19, 2041002.	1.8	3
18	SAAMBE-3D: Predicting Effect of Mutations on Protein-Protein Interactions. <i>International Journal of Molecular Sciences</i> , 2020, 21, 2563.	1.8	66

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19	A Newton-like iterative method implemented in the DelPhi for solving the nonlinear Poisson-Boltzmann equation. <i>Mathematical Biosciences and Engineering</i> , 2020, 17, 6259-6277.	1.0	0
20	DFMD: Fast and Effective DelPhiForce Steered Molecular Dynamics Approach to Model Ligand Approach Toward a Receptor: Application to Spermine Synthase Enzyme. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 74.	1.6	17
21	Modeling pKas of unfolded proteins to probe structural models of unfolded state. <i>Journal of Theoretical and Computational Chemistry</i> , 2019, 18, 1950020.	1.8	2
22	A super-Gaussian Poisson-Boltzmann model for electrostatic free energy calculation: smooth dielectric distribution for protein cavities and in both water and vacuum states. <i>Journal of Mathematical Biology</i> , 2019, 79, 631-672.	0.8	15
23	DelPhi Suite: New Developments and Review of Functionalities. <i>Journal of Computational Chemistry</i> , 2019, 40, 2502-2508.	1.5	38
24	Novel Genetic Markers for Early Detection of Elevated Breast Cancer Risk in Women. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4828.	1.8	3
25	Modeling Electrostatic Force in Protein-Protein Recognition. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 94.	1.6	22
26	A grid-based algorithm in conjunction with a gaussian-based model of atoms for describing molecular geometry. <i>Journal of Computational Chemistry</i> , 2019, 40, 1290-1304.	1.5	2
27	Structural Perspective on Revealing and Altering Molecular Functions of Genetic Variants Linked with Diseases. <i>International Journal of Molecular Sciences</i> , 2019, 20, 548.	1.8	20
28	Processivity vs. Beating: Comparing Cytoplasmic and Axonemal Dynein Microtubule Binding Domain Association with Microtubule. <i>International Journal of Molecular Sciences</i> , 2019, 20, 1090.	1.8	1
29	Three additional patients with EED-associated overgrowth: potential mutation hotspots identified?. <i>Journal of Human Genetics</i> , 2019, 64, 561-572.	1.1	16
30	PKAD: a database of experimentally measured pKa values of ionizable groups in proteins. Database: the <i>Journal of Biological Databases and Curation</i> , 2019, 2019, .	1.4	102
31	Modeling electrostatics in molecular biology: A tutorial of DelPhi and associated resources [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019, 1, .	2.2	5
32	Evaluation of performance of leading algorithms for variant pathogenicity predictions and designing a combinatory predictor method: application to Rett syndrome variants. <i>PeerJ</i> , 2019, 7, e8106.	0.9	10
33	Reproducing ensemble averaged electrostatics with Super-Gaussian-based smooth dielectric function: application to electrostatic component of binding energy of protein complexes. <i>Communications in Information and Systems</i> , 2019, 19, 405-423.	0.3	5
34	The capricious electrostatic force: Revealing the signaling pathway in integrin $\beta 2$ -I domain. <i>Journal of Theoretical and Computational Chemistry</i> , 2018, 17, 1840001.	1.8	3
35	Predicting protein-DNA binding free energy change upon missense mutations using modified MM/PBSA approach: SAMPDI webserver. <i>Bioinformatics</i> , 2018, 34, 779-786.	1.8	55
36	Reproducing the Ensemble Average Polar Solvation Energy of a Protein from a Single Structure: Gaussian-Based Smooth Dielectric Function for Macromolecular Modeling. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1020-1032.	2.3	15

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37	Key apoptotic genes APAF1 and CASP9 implicated in recurrent folate-resistant neural tube defects. <i>European Journal of Human Genetics</i> , 2018, 26, 420-427.	1.4	20
38	DelPhiPKa: Including salt in the calculations and enabling polar residues to titrate. <i>Proteins: Structure, Function and Bioinformatics</i> , 2018, 86, 1277-1283.	1.5	50
39	E-hooks provide guidance and a soft landing for the microtubule binding domain of dynein. <i>Scientific Reports</i> , 2018, 8, 13266.	1.6	21
40	Gaussian-Based Smooth Dielectric Function: A Surface-Free Approach for Modeling Macromolecular Binding in Solvents. <i>Frontiers in Molecular Biosciences</i> , 2018, 5, 25.	1.6	17
41	Computational Investigation of the Missense Mutations in DHCR7 Gene Associated with Smith-Lemli-Opitz Syndrome. <i>International Journal of Molecular Sciences</i> , 2018, 19, 141.	1.8	11
42	DelPhiForce, a tool for electrostatic force calculations: Applications to macromolecular binding. <i>Journal of Computational Chemistry</i> , 2017, 38, 584-593.	1.5	48
43	Treating ion distribution with Gaussian-based smooth dielectric function in DelPhi. <i>Journal of Computational Chemistry</i> , 2017, 38, 1974-1979.	1.5	30
44	A New DelPhi Feature for Modeling Electrostatic Potential around Proteins: Role of Bound Ions and Implications for Zeta-Potential. <i>Langmuir</i> , 2017, 33, 2283-2295.	1.6	16
45	Cytoskeletal-like Filaments of Ca ²⁺ -Calmodulin-Dependent Protein Kinase II Are Formed in a Regulated and Zn ²⁺ -Dependent Manner. <i>Biochemistry</i> , 2017, 56, 2149-2160.	1.2	7
46	Identification and characterization of a missense mutation in the O-linked ð ² -N-acetylglucosamine (O-GlcNAc) transferase gene that segregates with X-linked intellectual disability. <i>Journal of Biological Chemistry</i> , 2017, 292, 8948-8963.	1.6	87
47	Computational investigation of proton transfer, pKa shifts and pH-optimum of protein-DNA and protein-RNA complexes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 282-295.	1.5	20
48	Forces and Disease: Electrostatic force differences caused by mutations in kinesin motor domains can distinguish between disease-causing and non-disease-causing mutations. <i>Scientific Reports</i> , 2017, 7, 8237.	1.6	30
49	DelPhiForce web server: electrostatic forces and energy calculations and visualization. <i>Bioinformatics</i> , 2017, 33, 3661-3663.	1.8	44
50	SAAMBE: Webserver to Predict the Charge of Binding Free Energy Caused by Amino Acids Mutations. <i>International Journal of Molecular Sciences</i> , 2016, 17, 547.	1.8	59
51	Revealing the Effects of Missense Mutations Causing Snyder-Robinson Syndrome on the Stability and Dimerization of Spermine Synthase. <i>International Journal of Molecular Sciences</i> , 2016, 17, 77.	1.8	29
52	SAAFEC: Predicting the Effect of Single Point Mutations on Protein Folding Free Energy Using a Knowledge-Modified MM/PBSA Approach. <i>International Journal of Molecular Sciences</i> , 2016, 17, 512.	1.8	72
53	Cytoplasmic dynein binding, run length, and velocity are guided by long-range electrostatic interactions. <i>Scientific Reports</i> , 2016, 6, 31523.	1.6	44
54	Cofactors-loaded quaternary structure of lysine-specific demethylase 5C (KDM5C) protein: Computational model. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 1797-1809.	1.5	7

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55	Electrostatic component of binding energy: Interpreting predictions from poisson-boltzmann equation and modeling protocols. <i>Journal of Computational Chemistry</i> , 2016, 37, 2495-2507.	1.5	17
56	Multiscale method for modeling binding phenomena involving large objects: application to kinesin motor domains motion along microtubules. <i>Scientific Reports</i> , 2016, 6, 23249.	1.6	30
57	Investigating the linkage between disease-causing amino acid variants and their effect on protein stability and binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 232-239.	1.5	46
58	Binding Analysis of Methyl-CpG Binding Domain of MeCP2 and Rett Syndrome Mutations. <i>ACS Chemical Biology</i> , 2016, 11, 2706-2715.	1.6	50
59	DelPhiPKa web server: predicting p <i>K</i> a of proteins, RNAs and DNAs. <i>Bioinformatics</i> , 2016, 32, 614-615.	1.8	98
60	Navigating through Genomics Data to Deliver Testable Predictions. <i>Human Mutation</i> , 2015, 36, v-v.	1.1	1
61	p <i>K</i> a predictions for proteins, RNA, and DNA with the Gaussian dielectric function using DelPhi p <i>K</i> a. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 2186-2197.	1.5	104
62	Statistical investigation of surface bound ions and further development of BION server to include p <i>H</i> and salt dependence. <i>Journal of Computational Chemistry</i> , 2015, 36, 2381-2393.	1.5	14
63	Mutations in the KDM5C ARID Domain and Their Plausible Association with Syndromic Claes-Jensen-Type Disease. <i>International Journal of Molecular Sciences</i> , 2015, 16, 27270-27287.	1.8	21
64	On the energy components governing molecular recognition in the framework of continuum approaches. <i>Frontiers in Molecular Biosciences</i> , 2015, 2, 5.	1.6	36
65	Structural, Dynamical, and Energetical Consequences of Rett Syndrome Mutation R133C in MeCP2. <i>Computational and Mathematical Methods in Medicine</i> , 2015, 2015, 1-9.	0.7	14
66	Structural and physico-chemical effects of disease and non-disease nsSNPs on proteins. <i>Current Opinion in Structural Biology</i> , 2015, 32, 18-24.	2.6	165
67	ZC4H2, an XLID gene, is required for the generation of a specific subset of CNS interneurons. <i>Human Molecular Genetics</i> , 2015, 24, 4848-4861.	1.4	48
68	On Human Disease-Causing Amino Acid Variants: Statistical Study of Sequence and Structural Patterns. <i>Human Mutation</i> , 2015, 36, 524-534.	1.1	122
69	Impact of Rett Syndrome Mutations on MeCP2 MBD Stability. <i>Biochemistry</i> , 2015, 54, 6357-6368.	1.2	30
70	Predicting Binding Free Energy Change Caused by Point Mutations with Knowledge-Modified MM/PBSA Method. <i>PLoS Computational Biology</i> , 2015, 11, e1004276.	1.5	94
71	Rational Design of Small-Molecule Stabilizers of Spermine Synthase Dimer by Virtual Screening and Free Energy-Based Approach. <i>PLoS ONE</i> , 2014, 9, e110884.	1.1	20
72	Chronic Beryllium Disease: Revealing the Role of Beryllium Ion and Small Peptides Binding to HLA-DP2. <i>PLoS ONE</i> , 2014, 9, e111604.	1.1	14

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73	Advances in Human Biology: Combining Genetics and Molecular Biophysics to Pave the Way for Personalized Diagnostics and Medicine. <i>Advances in Biology</i> , 2014, 2014, 1-16.	1.2	10
74	A Novel p.Leu(381)Phe Mutation in Presenilin 1 is Associated with Very Early Onset and Unusually Fast Progressing Dementia as well as Lysosomal Inclusions Typically Seen in Kufs Disease. <i>Journal of Alzheimer's Disease</i> , 2014, 39, 23-27.	1.2	21
75	On the electrostatic properties of homodimeric proteins. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1440007.	1.8	12
76	Computational and Experimental Approaches to Reveal the Effects of Single Nucleotide Polymorphisms with Respect to Disease Diagnostics. <i>International Journal of Molecular Sciences</i> , 2014, 15, 9670-9717.	1.8	31
77	On the modeling of polar component of solvation energy using smooth Gaussian-based dielectric function. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1440002.	1.8	36
78	ProBLM Web Server: Protein and Membrane Placement and Orientation Package. <i>Computational and Mathematical Methods in Medicine</i> , 2014, 2014, 1-7.	0.7	16
79	Modeling the electrostatic potential of asymmetric lipopolysaccharide membranes: The MEMPOT algorithm implemented in DelPhi. <i>Journal of Computational Chemistry</i> , 2014, 35, 1418-1429.	1.5	17
80	A mutation in a ganglioside biosynthetic enzyme, ST3GAL5, results in salt & pepper syndrome, a neurocutaneous disorder with altered glycolipid and glycoprotein glycosylation. <i>Human Molecular Genetics</i> , 2014, 23, 418-433.	1.4	144
81	Predicting the Impact of Missense Mutations on Protein-Protein Binding Affinity. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 1770-1780.	2.3	102
82	Ion binding to biological macromolecules. <i>Asian Journal of Physics</i> , 2014, 23, 735-744.	0.0	9
83	Protonation and pK changes in protein-ligand binding. <i>Quarterly Reviews of Biophysics</i> , 2013, 46, 181-209.	2.4	151
84	Molecular Mechanisms of Disease-Causing Missense Mutations. <i>Journal of Molecular Biology</i> , 2013, 425, 3919-3936.	2.0	242
85	A Y328C missense mutation in spermine synthase causes a mild form of Snyder-Robinson syndrome. <i>Human Molecular Genetics</i> , 2013, 22, 3789-3797.	1.4	31
86	BION web server: predicting non-specifically bound surface ions. <i>Bioinformatics</i> , 2013, 29, 805-806.	1.8	15
87	Understanding Molecular Effects of Naturally Occurring Genetic Differences. <i>Journal of Molecular Biology</i> , 2013, 425, 3911-3913.	2.0	17
88	Continuous development of schemes for parallel computing of the electrostatics in biological systems: Implementation in DelPhi. <i>Journal of Computational Chemistry</i> , 2013, 34, 1949-1960.	1.5	26
89	On the Dielectric Constant of Proteins: Smooth Dielectric Function for Macromolecular Modeling and Its Implementation in DelPhi. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2126-2136.	2.3	446
90	A rational free energy-based approach to understanding and targeting disease-causing missense mutations. <i>Journal of the American Medical Informatics Association: JAMIA</i> , 2013, 20, 643-651.	2.2	18

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91	Progress in developing Poisson-Boltzmann equation solvers. Computational and Mathematical Biophysics, 2013, 1, 42-62.	0.6	29
92	Enhancing Human Spermine Synthase Activity by Engineered Mutations. PLoS Computational Biology, 2013, 9, e1002924.	1.5	19
93	In Silico Investigation of pH-Dependence of Prolactin and Human Growth Hormone Binding to Human Prolactin Receptor. Communications in Computational Physics, 2013, 13, 207-222.	0.7	20
94	Between Algorithm and Model: Different Molecular Surface Definitions for the Poisson-Boltzmann Based Electrostatic Characterization of Biomolecules in Solution. Communications in Computational Physics, 2013, 13, 61-89.	0.7	46
95	Using DelPhi Capabilities to Mimic Protein's Conformational Reorganization with Amino Acid Specific Dielectric Constants. Communications in Computational Physics, 2013, 13, 13-30.	0.7	23
96	The Role of Protonation States in Ligand-Receptor Recognition and Binding. Current Pharmaceutical Design, 2013, 19, 4182-4190.	0.9	77
97	DelPhi Web Server: A Comprehensive Online Suite for Electrostatic Calculations of Biological Macromolecules and Their Complexes. Communications in Computational Physics, 2013, 13, 269-284.	0.7	52
98	Cancer Missense Mutations Alter Binding Properties of Proteins and Their Interaction Networks. PLoS ONE, 2013, 8, e66273.	1.1	102
99	An X-linked channelopathy with cardiomegaly due to a CLIC2 mutation enhancing ryanodine receptor channel activity. Human Molecular Genetics, 2012, 21, 4497-4507.	1.4	84
100	Analyzing Effects of Naturally Occurring Missense Mutations. Computational and Mathematical Methods in Medicine, 2012, 2012, 1-15.	0.7	111
101	DelPhi web server v2: incorporating atomic-style geometrical figures into the computational protocol. Bioinformatics, 2012, 28, 1655-1657.	1.8	43
102	Predicting Nonspecific Ion Binding Using DelPhi. Biophysical Journal, 2012, 102, 2885-2893.	0.2	27
103	Protein Nano-Object Integrator (ProNOI) for generating atomic style objects for molecular modeling. BMC Structural Biology, 2012, 12, 31.	2.3	4
104	DelPhi: a comprehensive suite for DelPhi software and associated resources. BMC Biophysics, 2012, 5, 9.	4.4	315
105	Predicting folding free energy changes upon single point mutations. Bioinformatics, 2012, 28, 664-671.	1.8	85
106	Highly efficient and exact method for parallelization of grid-based algorithms and its implementation in DelPhi. Journal of Computational Chemistry, 2012, 33, 1960-1966.	1.5	49
107	On the role of electrostatics in protein-protein interactions. Physical Biology, 2011, 8, 035001.	0.8	139
108	In Silico and In Vitro Investigations of the Mutability of Disease-Causing Missense Mutation Sites in Spermine Synthase. PLoS ONE, 2011, 6, e20373.	1.1	53

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109	<i>In silico</i> modeling of p <i>H</i> optimum of protein-protein binding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 925-936.	1.5	49
110	A missense mutation in <i>CLIC2</i> associated with intellectual disability is predicted by <i>in silico</i> modeling to affect protein stability and dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 2444-2454.	1.5	79
111	Developing hybrid approaches to predict p <i>K_a</i> values of ionizable groups. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3389-3399.	1.5	36
112	Progress in the prediction of p <i>K_a</i> values in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 3260-3275.	1.5	229
113	Structural assessment of the effects of Amino Acid Substitutions on protein stability and protein-protein interaction. <i>International Journal of Computational Biology and Drug Design</i> , 2010, 3, 334.	0.3	39
114	Computational analysis of missense mutations causing Snyder-Robinson syndrome. <i>Human Mutation</i> , 2010, 31, 1043-1049.	1.1	85
115	On the p <i>H</i> optimum of activity and stability of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 2699-2706.	1.5	228
116	Modeling Effects of Human Single Nucleotide Polymorphisms on Protein-Protein Interactions. <i>Biophysical Journal</i> , 2009, 96, 2178-2188.	0.2	117
117	On the electrostatic component of protein-protein binding free energy. <i>PMC Biophysics</i> , 2008, 1, 2.	2.2	49
118	Homology-based modeling of 3D structures of protein-protein complexes using alignments of modified sequence profiles. <i>International Journal of Biological Macromolecules</i> , 2008, 43, 198-208.	3.6	39
119	Editorial [Protein-Protein Interactions Guest Editor: Emil Alexov]. <i>Current Pharmaceutical Biotechnology</i> , 2008, 9, 55-56.	0.9	10
120	Calculating the Protonation States of Proteins and Small Molecules: Implications to Ligand-Receptor Interactions. <i>Current Computer-Aided Drug Design</i> , 2008, 4, 169-179.	0.8	24
121	PROTCOM: searchable database of protein complexes enhanced with domain-domain structures. <i>Nucleic Acids Research</i> , 2007, 35, D575-D579.	6.5	43
122	Calculation of p <i>K_a</i> in RNA: On the Structural Origins and Functional Roles of Protonated Nucleotides. <i>Journal of Molecular Biology</i> , 2007, 366, 1475-1496.	2.0	137
123	Predicting interacting and interfacial residues using continuous sequence segments. <i>International Journal of Biological Macromolecules</i> , 2007, 41, 615-623.	3.6	4
124	Poisson-Boltzmann Calculations of Nonspecific Salt Effects on Protein-Protein Binding Free Energies. <i>Biophysical Journal</i> , 2007, 92, 1891-1899.	0.2	96
125	Optimization of Electrostatic Interactions in Protein-Protein Complexes. <i>Biophysical Journal</i> , 2007, 93, 3340-3352.	0.2	55
126	Structural and functional consequences of single amino acid substitutions in the pyrimidine base binding pocket of <i>Escherichia coli</i> CMP kinase. <i>FEBS Journal</i> , 2007, 274, 3363-3373.	2.2	17

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127	Electrostatic Properties of Protein-Protein Complexes. <i>Biophysical Journal</i> , 2006, 91, 1724-1736.	0.2	81
128	Characterizing a Partially Folded Intermediate of the Villin Headpiece Domain Under Non-denaturing Conditions: Contribution of His41 to the pH-dependent Stability of the N-terminal Subdomain. <i>Journal of Molecular Biology</i> , 2006, 355, 1078-1094.	2.0	63
129	Predicting 3D structures of transient protein-protein complexes by homology. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2006, 1764, 1498-1511.	1.1	21
130	Calculating proton uptake/release and binding free energy taking into account ionization and conformation changes induced by protein-inhibitor association: Application to plasmeprin, cathepsin D and endothiapsin-pepstatin complexes. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 56, 572-584.	1.5	48
131	Numerical calculations of the pH of maximal protein stability. <i>FEBS Journal</i> , 2003, 271, 173-185.	0.2	76
132	Using multiple structure alignments, fast model building, and energetic analysis in fold recognition and homology modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 53, 430-435.	1.5	290
133	On the Role of Structural Information in Remote Homology Detection and Sequence Alignment: New Methods Using Hybrid Sequence Profiles. <i>Journal of Molecular Biology</i> , 2003, 334, 1043-1062.	2.0	84
134	Rapid grid-based construction of the molecular surface and the use of induced surface charge to calculate reaction field energies: Applications to the molecular systems and geometric objects. <i>Journal of Computational Chemistry</i> , 2002, 23, 128-137.	1.5	631
135	Role of the protein side-chain fluctuations on the strength of pair-wise electrostatic interactions: Comparing experimental with computed pKas. <i>Proteins: Structure, Function and Bioinformatics</i> , 2002, 50, 94-103.	1.5	62
136	pH-dependent interactions of Apolipoprotein III with a lipid disk. <i>Journal of Theoretical and Computational Chemistry</i> , 0, , 2042004.	1.8	0