Emil Alexov

List of Publications by Year
in descending order

136	7,436	53794 45	62596 80
papers	citations	h-index	g-index

140	140	140	7923
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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. Journal of Computational Chemistry, 2002, 23, 128-137.	3.3	631
2	On the Dielectric â€œConstantâ€•of Proteins: Smooth Dielectric Function for Macromolecular Modeling and Its Implementation in DelPhi. Journal of Chemical Theory and Computation, 2013, 9, 2126-2136.	5.3	446
3	DelPhi: a comprehensive suite for DelPhi software and associated resources. BMC Biophysics, 2012, 5, 9.	4.4	315
4	Using multiple structure alignments, fast model building, and energetic analysis in fold recognition and homology modeling. Proteins: Structure, Function and Bioinformatics, 2003, 53, 430-435.	2.6	290
5	Molecular Mechanisms of Disease-Causing Missense Mutations. Journal of Molecular Biology, 2013, 425, 3919-3936.	4.2	242
6	Progress in the prediction of pK_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
7	On the pHâ€optimum of activity and stability of proteins. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2699-2706.	2.6	228
8	Structural and physico-chemical effects of disease and non-disease nsSNPs on proteins. Current Opinion in Structural Biology, 2015, 32, 18-24.	5.7	165
9	Protonation and pK changes in proteinâ€“ligand binding. Quarterly Reviews of Biophysics, 2013, 46, 181-209.	5.7	151
10	A mutation in a ganglioside biosynthetic enzyme, ST3GAL5, results in salt & pepper syndrome, a neurocutaneous disorder with altered glycolipid and glycoprotein glycosylation. Human Molecular Genetics, 2014, 23, 418-433.	2.9	144
11	On the role of electrostatics in proteinâ€“protein interactions. Physical Biology, 2011, 8, 035001.	1.8	139
12	Calculation of pKas in RNA: On the Structural Origins and Functional Roles of Protonated Nucleotides. Journal of Molecular Biology, 2007, 366, 1475-1496.	4.2	137
13	On Human Disease-Causing Amino Acid Variants: Statistical Study of Sequence and Structural Patterns. Human Mutation, 2015, 36, 524-534.	2.5	122
14	Modeling Effects of Human Single Nucleotide Polymorphisms on Protein-Protein Interactions. Biophysical Journal, 2009, 96, 2178-2188.	0.5	117
15	Analyzing Effects of Naturally Occurring Missense Mutations. Computational and Mathematical Methods in Medicine, 2012, 2012, 1-15.	1.3	111
16	pKa predictions for proteins, <scp>RNA</scp>s, and <scp>DNA</scp>s with the Gaussian dielectric function using DelPhi pKa. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2186-2197.	2.6	104
17	Predicting the Impact of Missense Mutations on Proteinâ€“Protein Binding Affinity. Journal of Chemical Theory and Computation, 2014, 10, 1770-1780.	5.3	102
18	PKAD: a database of experimentally measured pKa values of ionizable groups in proteins. Database: the Journal of Biological Databases and Curation, 2019, 2019, .	3.0	102

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19	Cancer Missense Mutations Alter Binding Properties of Proteins and Their Interaction Networks. PLoS ONE, 2013, 8, e66273.	2.5	102
20	DelPhiPKa web server: predicting pKa of proteins, RNAs and DNAs. Bioinformatics, 2016, 32, 614-615.	4.1	98
21	Poisson-Boltzmann Calculations of Nonspecific Salt Effects on Protein-Protein Binding Free Energies. Biophysical Journal, 2007, 92, 1891-1899.	0.5	96
22	Predicting Binding Free Energy Change Caused by Point Mutations with Knowledge-Modified MM/PBSA Method. PLoS Computational Biology, 2015, 11, e1004276.	3.2	94
23	Identification and characterization of a missense mutation in the O-linked Î²-N-acetylglucosamine (O-GlcNAc) transferase gene that segregates with X-linked intellectual disability. Journal of Biological Chemistry, 2017, 292, 8948-8963.	3.4	87
24	Computational analysis of missense mutations causing Snyder-Robinson syndrome. Human Mutation, 2010, 31, 1043-1049.	2.5	85
25	Predicting folding free energy changes upon single point mutations. Bioinformatics, 2012, 28, 664-671.	4.1	85
26	On the Role of Structural Information in Remote Homology Detection and Sequence Alignment: New Methods Using Hybrid Sequence Profiles. Journal of Molecular Biology, 2003, 334, 1043-1062.	4.2	84
27	An X-linked channelopathy with cardiomegaly due to a CLIC2 mutation enhancing ryanodine receptor channel activity. Human Molecular Genetics, 2012, 21, 4497-4507.	2.9	84
28	Electrostatic Properties of Protein-Protein Complexes. Biophysical Journal, 2006, 91, 1724-1736.	0.5	81
29	A missense mutation in CLIC2 associated with intellectual disability is predicted by in silico modeling to affect protein stability and dynamics. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2444-2454.	2.6	79
30	The Role of Protonation States in Ligand-Receptor Recognition and Binding. Current Pharmaceutical Design, 2013, 19, 4182-4190.	1.9	77
31	Numerical calculations of the pH of maximal protein stability. FEBS Journal, 2003, 271, 173-185.	0.2	76
32	SAAFEC: Predicting the Effect of Single Point Mutations on Protein Folding Free Energy Using a Knowledge-Modified MM/PBSA Approach. International Journal of Molecular Sciences, 2016, 17, 512.	4.1	72
33	SAAMBE-3D: Predicting Effect of Mutations on Proteinâ€“Protein Interactions. International Journal of Molecular Sciences, 2020, 21, 2563.	4.1	66
34	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. Journal of Molecular Biology, 2006, 355, 1078-1094.	4.2	63
35	SAAFEC-SEQ: A Sequence-Based Method for Predicting the Effect of Single Point Mutations on Protein Thermodynamic Stability. International Journal of Molecular Sciences, 2021, 22, 606.	4.1	63
36	Role of the protein side-chain fluctuations on the strength of pair-wise electrostatic interactions: Comparing experimental with computed pKas. Proteins: Structure, Function and Bioinformatics, 2002, 50, 94-103.	2.6	62

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37	SAAMBE: Webserver to Predict the Charge of Binding Free Energy Caused by Amino Acids Mutations. International Journal of Molecular Sciences, 2016, 17, 547.	4.1	59
38	Optimization of Electrostatic Interactions in Protein-Protein Complexes. Biophysical Journal, 2007, 93, 3340-3352.	0.5	55
39	Predicting proteinâ€“DNA binding free energy change upon missense mutations using modified MM/PBSA approach: SAMPDI webserver. Bioinformatics, 2018, 34, 779-786.	4.1	55
40	In Silico and In Vitro Investigations of the Mutability of Disease-Causing Missense Mutation Sites in Spermine Synthase. PLoS ONE, 2011, 6, e20373.	2.5	53
41	DelPhi Web Server: A Comprehensive Online Suite for Electrostatic Calculations of Biological Macromolecules and Their Complexes. Communications in Computational Physics, 2013, 13, 269-284.	1.7	52
42	Binding Analysis of Methyl-CpG Binding Domain of MeCP2 and Rett Syndrome Mutations. ACS Chemical Biology, 2016, 11, 2706-2715.	3.4	50
43	DelPhiPKa: Including salt in the calculations and enabling polar residues to titrate. Proteins: Structure, Function and Bioinformatics, 2018, 86, 1277-1283.	2.6	50
44	On the electrostatic component of protein-protein binding free energy. PMC Biophysics, 2008, 1, 2.	2.3	49
45	In silico modeling of pHâ€optimum of proteinâ€“protein binding. Proteins: Structure, Function and Bioinformatics, 2011, 79, 925-936.	2.6	49
46	Highly efficient and exact method for parallelization of gridâ€based algorithms and its implementation in DelPhi. Journal of Computational Chemistry, 2012, 33, 1960-1966.	3.3	49
47	Calculating proton uptake/release and binding free energy taking into account ionization and conformation changes induced by protein-inhibitor association: Application to plasmepsin, cathepsin D and endothiapepsin-pepstatin complexes. Proteins: Structure, Function and Bioinformatics, 2004, 56, 572-584.	2.6	48
48	ZC4H2, an XLID gene, is required for the generation of a specific subset of CNS interneurons. Human Molecular Genetics, 2015, 24, 4848-4861.	2.9	48
49	DelPhiForce, a tool for electrostatic force calculations: Applications to macromolecular binding. Journal of Computational Chemistry, 2017, 38, 584-593.	3.3	48
50	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.	1.7	46
51	Investigating the linkage between disease-causing amino acid variants and their effect on protein stability and binding. Proteins: Structure, Function and Bioinformatics, 2016, 84, 232-239.	2.6	46
52	Cytoplasmic dynein binding, run length, and velocity are guided by long-range electrostatic interactions. Scientific Reports, 2016, 6, 31523.	3.3	44
53	DelPhiForce web server: electrostatic forces and energy calculations and visualization. Bioinformatics, 2017, 33, 3661-3663.	4.1	44
54	PROTCOM: searchable database of protein complexes enhanced with domain-domain structures. Nucleic Acids Research, 2007, 35, D575-D579.	14.5	43

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55	DelPhi web server v2: incorporating atomic-style geometrical figures into the computational protocol. Bioinformatics, 2012, 28, 1655-1657.	4.1	43
56	Homology-based modeling of 3D structures of proteinâ€“protein complexes using alignments of modified sequence profiles. International Journal of Biological Macromolecules, 2008, 43, 198-208.	7.5	39
57	Structural assessment of the effects of Amino Acid Substitutions on protein stability and protein protein interaction. International Journal of Computational Biology and Drug Design, 2010, 3, 334.	0.3	39
58	DelPhi Suite: New Developments and Review of Functionalities. Journal of Computational Chemistry, 2019, 40, 2502-2508.	3.3	38
59	Mutations in FAM50A suggest that Armfield XLID syndrome is a spliceosomopathy. Nature Communications, 2020, 11, 3698.	12.8	38
60	Developing hybrid approaches to predict pK_avalues of ionizable groups. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3389-3399.	2.6	36
61	On the modeling of polar component of solvation energy using smooth Gaussian-based dielectric function. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440002.	1.8	36
62	On the energy components governing molecular recognition in the framework of continuum approaches. Frontiers in Molecular Biosciences, 2015, 2, 5.	3.5	36
63	A Y328C missense mutation in spermine synthase causes a mild form of Snyderâ€“Robinson syndrome. Human Molecular Genetics, 2013, 22, 3789-3797.	2.9	31
64	Computational and Experimental Approaches to Reveal the Effects of Single Nucleotide Polymorphisms with Respect to Disease Diagnostics. International Journal of Molecular Sciences, 2014, 15, 9670-9717.	4.1	31
65	Impact of Rett Syndrome Mutations on MeCP2 MBD Stability. Biochemistry, 2015, 54, 6357-6368.	2.5	30
66	Multiscale method for modeling binding phenomena involving large objects: application to kinesin motor domains motion along microtubules. Scientific Reports, 2016, 6, 23249.	3.3	30
67	Treating ion distribution with Gaussian-based smooth dielectric function in DelPhi. Journal of Computational Chemistry, 2017, 38, 1974-1979.	3.3	30
68	Forces and Disease: Electrostatic force differences caused by mutations in kinesin motor domains can distinguish between disease-causing and non-disease-causing mutations. Scientific Reports, 2017, 7, 8237.	3.3	30
69	Progress in developing Poisson-Boltzmann equation solvers. Computational and Mathematical Biophysics, 2013, 1, 42-62.	1.1	29
70	Revealing the Effects of Missense Mutations Causing Snyder-Robinson Syndrome on the Stability and Dimerization of Spermine Synthase. International Journal of Molecular Sciences, 2016, 17, 77.	4.1	29
71	Predicting Nonspecific Ion Binding Using DelPhi. Biophysical Journal, 2012, 102, 2885-2893.	0.5	27
72	Continuous development of schemes for parallel computing of the electrostatics in biological systems: Implementation in DelPhi. Journal of Computational Chemistry, 2013, 34, 1949-1960.	3.3	26

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73	Calculating the Protonation States of Proteins and Small Molecules: Implications to Ligand-Receptor Interactions. Current Computer-Aided Drug Design, 2008, 4, 169-179.	1.2	24
74	Using DelPhi Capabilities to Mimic Proteinâ€™s Conformational Reorganization with Amino Acid Specific Dielectric Constants. Communications in Computational Physics, 2013, 13, 13-30.	1.7	23
75	Modeling Electrostatic Force in Protein-Protein Recognition. Frontiers in Molecular Biosciences, 2019, 6, 94.	3.5	22
76	Predicting 3D structures of transient proteinâ€“protein complexes by homology. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2006, 1764, 1498-1511.	2.3	21
77	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. Journal of Alzheimer's Disease, 2014, 39, 23-27.	2.6	21
78	Mutations in the KDM5C ARID Domain and Their Plausible Association with Syndromic Claes-Jensen-Type Disease. International Journal of Molecular Sciences, 2015, 16, 27270-27287.	4.1	21
79	E-hooks provide guidance and a soft landing for the microtubule binding domain of dynein. Scientific Reports, 2018, 8, 13266.	3.3	21
80	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.	1.7	20
81	Rational Design of Small-Molecule Stabilizers of Spermine Synthase Dimer by Virtual Screening and Free Energy-Based Approach. PLoS ONE, 2014, 9, e110884.	2.5	20
82	Computational investigation of proton transfer, pKa shifts and pH-optimum of protein-DNA and protein-RNA complexes. Proteins: Structure, Function and Bioinformatics, 2017, 85, 282-295.	2.6	20
83	Key apoptotic genes APAF1 and CASP9 implicated in recurrent folate-resistant neural tube defects. European Journal of Human Genetics, 2018, 26, 420-427.	2.8	20
84	Structural Perspective on Revealing and Altering Molecular Functions of Genetic Variants Linked with Diseases. International Journal of Molecular Sciences, 2019, 20, 548.	4.1	20
85	Enhancing Human Spermine Synthase Activity by Engineered Mutations. PLoS Computational Biology, 2013, 9, e1002924.	3.2	19
86	A rational free energy-based approach to understanding and targeting disease-causing missense mutations. Journal of the American Medical Informatics Association: JAMIA, 2013, 20, 643-651.	4.4	18
87	Structural and functional consequences of single amino acid substitutions in the pyrimidine base binding pocket of Escherichia coli CMP kinase. FEBS Journal, 2007, 274, 3363-3373.	4.7	17
88	Understanding Molecular Effects of Naturally Occurring Genetic Differences. Journal of Molecular Biology, 2013, 425, 3911-3913.	4.2	17
89	Modeling the electrostatic potential of asymmetric lipopolysaccharide membranes: The MEMPOT algorithm implemented in DelPhi. Journal of Computational Chemistry, 2014, 35, 1418-1429.	3.3	17
90	Electrostatic component of binding energy: Interpreting predictions from poissonâ€“boltzmann equation and modeling protocols. Journal of Computational Chemistry, 2016, 37, 2495-2507.	3.3	17

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91	Gaussian-Based Smooth Dielectric Function: A Surface-Free Approach for Modeling Macromolecular Binding in Solvents. Frontiers in Molecular Biosciences, 2018, 5, 25.	3.5	17
92	DFMD: Fast and Effective DelPhiForce Steered Molecular Dynamics Approach to Model Ligand Approach Toward a Receptor: Application to Spermine Synthase Enzyme. Frontiers in Molecular Biosciences, 2019, 6, 74.	3.5	17
93	SAAMBE-SEQ: a sequence-based method for predicting mutation effect on proteinâ€“protein binding affinity. Bioinformatics, 2021, 37, 992-999.	4.1	17
94	ProBLM Web Server: Protein and Membrane Placement and Orientation Package. Computational and Mathematical Methods in Medicine, 2014, 2014, 1-7.	1.3	16
95	A New DelPhi Feature for Modeling Electrostatic Potential around Proteins: Role of Bound Ions and Implications for Zeta-Potential. Langmuir, 2017, 33, 2283-2295.	3.5	16
96	Three additional patients with EED-associated overgrowth: potential mutation hotspots identified?. Journal of Human Genetics, 2019, 64, 561-572.	2.3	16
97	BION web server: predicting non-specifically bound surface ions. Bioinformatics, 2013, 29, 805-806.	4.1	15
98	Reproducing the Ensemble Average Polar Solvation Energy of a Protein from a Single Structure: Gaussian-Based Smooth Dielectric Function for Macromolecular Modeling. Journal of Chemical Theory and Computation, 2018, 14, 1020-1032.	5.3	15
99	A super-Gaussian Poissonâ€“Boltzmann model for electrostatic free energy calculation: smooth dielectric distribution for protein cavities and in both water and vacuum states. Journal of Mathematical Biology, 2019, 79, 631-672.	1.9	15
100	Chronic Beryllium Disease: Revealing the Role of Beryllium Ion and Small Peptides Binding to HLA-DP2. PLoS ONE, 2014, 9, e111604.	2.5	14
101	Statistical investigation of surface bound ions and further development of <scp>BION</scp> server to include p<scp>H</scp> and salt dependence. Journal of Computational Chemistry, 2015, 36, 2381-2393.	3.3	14
102	Structural, Dynamical, and Energetical Consequences of Rett Syndrome Mutation R133C in MeCP2. Computational and Mathematical Methods in Medicine, 2015, 2015, 1-9.	1.3	14
103	On the electrostatic properties of homodimeric proteins. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440007.	1.8	12
104	Computational Investigation of the Missense Mutations in DHCR7 Gene Associated with Smith-Lemli-Opitz Syndrome. International Journal of Molecular Sciences, 2018, 19, 141.	4.1	11
105	Editorial [Protein-Protein Interactions Guest Editor: Emil Alexov]. Current Pharmaceutical Biotechnology, 2008, 9, 55-56.	1.6	10
106	Advances in Human Biology: Combining Genetics and Molecular Biophysics to Pave the Way for Personalized Diagnostics and Medicine. Advances in Biology, 2014, 2014, 1-16.	1.2	10
107	Evaluation of performance of leading algorithms for variant pathogenicity predictions and designing a combinatory predictor method: application to Rett syndrome variants. PeerJ, 2019, 7, e8106.	2.0	10
108	Ion binding to biological macromolecules. Asian Journal of Physics, 2014, 23, 735-744.	0.2	9

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109	Proteinâ€“Protein Binding Free Energy Predictions with the MM/PBSA Approach Complemented with the Gaussian-Based Method for Entropy Estimation. ACS Omega, 2022, 7, 11057-11067.	3.5	9
110	Capturing the Effects of Explicit Waters in Implicit Electrostatics Modeling: Qualitative Justification of Gaussian-Based Dielectric Models in DelPhi. Journal of Chemical Information and Modeling, 2020, 60, 2229-2246.	5.4	8
111	SAMPDI-3D: predicting the effects of protein and DNA mutations on proteinâ€“DNA interactions. Bioinformatics, 2021, 37, 3760-3765.	4.1	8
112	Cofactors-loaded quaternary structure of lysine-specific demethylase 5C (KDM5C) protein: Computational model. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1797-1809.	2.6	7
113	Cytoskeletal-like Filaments of Ca²⁺-Calmodulin-Dependent Protein Kinase II Are Formed in a Regulated and Zn²⁺-Dependent Manner. Biochemistry, 2017, 56, 2149-2160.	2.5	7
114	An Ensemble Approach to Predict the Pathogenicity of Synonymous Variants. Genes, 2020, 11, 1102.	2.4	6
115	On regularization of charge singularities in solving the Poisson-Boltzmann equation with a smooth solute-solvent boundary. Mathematical Biosciences and Engineering, 2021, 18, 1370-1405.	1.9	6
116	Increased p53 signaling impairs neural differentiation in HUWE1-promoted intellectual disabilities. Cell Reports Medicine, 2021, 2, 100240.	6.5	5
117	Modeling electrostatics in molecular biology: A tutorial of DelPhi and associated resources [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	6.4	5
118	BION-2: Predicting Positions of Non-Specifically Bound Ions on Protein Surface by a Gaussian-Based Treatment of Electrostatics. International Journal of Molecular Sciences, 2021, 22, 272.	4.1	5
119	Reproducing ensemble averaged electrostatics with Super-Gaussian-based smooth dielectric function: application to electrostatic component of binding energy of protein complexes. Communications in Information and Systems, 2019, 19, 405-423.	0.5	5
120	Predicting interacting and interfacial residues using continuous sequence segments. International Journal of Biological Macromolecules, 2007, 41, 615-623.	7.5	4
121	Protein Nano-Object Integrator (ProNOI) for generating atomic style objects for molecular modeling. BMC Structural Biology, 2012, 12, 31.	2.3	4
122	pH-Dependent Interactions of Apolipophorin-III with a Lipid Disk. Journal of Computational Biophysics and Chemistry, 2021, 20, 153-164.	1.7	4
123	A regularization approach for solving the super-Gaussian Poisson-Boltzmann model with heterogeneous dielectric functions. Journal of Computational Physics, 2022, 464, 111340.	3.8	4
124	The capricious electrostatic force: Revealing the signaling pathway in integrin Î±2-I domain. Journal of Theoretical and Computational Chemistry, 2018, 17, 1840001.	1.8	3
125	Novel Genetic Markers for Early Detection of Elevated Breast Cancer Risk in Women. International Journal of Molecular Sciences, 2019, 20, 4828.	4.1	3
126	In-silico analysis to identify the role of MEN1 missense mutations in breast cancer. Journal of Theoretical and Computational Chemistry, 2020, 19, 2041002.	1.8	3

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127	Opioid Addiction and Opioid Receptor Dimerization: Structural Modeling of the OPRD1 and OPRM1 Heterodimer and Its Signaling Pathways. International Journal of Molecular Sciences, 2021, 22, 10290.	4.1	3
128	Modeling pKas of unfolded proteins to probe structural models of unfolded state. Journal of Theoretical and Computational Chemistry, 2019, 18, 1950020.	1.8	2
129	A gridâ€based algorithm in conjunction with a gaussianâ€based model of atoms for describing molecular geometry. Journal of Computational Chemistry, 2019, 40, 1290-1304.	3.3	2
130	Computational chemistry methods to investigate the effects caused by DNA variants linked with disease. Journal of Theoretical and Computational Chemistry, 2020, 19, 1930001.	1.8	2
131	Ab-initio binding of barnaseâ€“barstar with DelPhiForce steered Molecular Dynamics (DFMD) approach. Journal of Theoretical and Computational Chemistry, 2020, 19, 2050016.	1.8	2
132	Computational Investigation of the pH Dependence of Stability of Melanosome Proteins: Implication for Melanosome formation and Disease. International Journal of Molecular Sciences, 2021, 22, 8273.	4.1	2
133	Navigating through Genomics Data to Deliver Testable Predictions. Human Mutation, 2015, 36, v-v.	2.5	1
134	Processivity vs. Beating: Comparing Cytoplasmic and Axonemal Dynein Microtubule Binding Domain Association with Microtubule. International Journal of Molecular Sciences, 2019, 20, 1090.	4.1	1
135	A Newton-like iterative method implemented in the DelPhi for solving the nonlinear Poisson-Boltzmann equation. Mathematical Biosciences and Engineering, 2020, 17, 6259-6277.	1.9	0
136	pH-dependent interactions of Apolipophorin-III with a lipid disk. Journal of Theoretical and Computational Chemistry, 0, , 2042004.	1.8	0