Sergei Grudinin

List of Publications by Year
in descending order

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67	2,047	279701	289141
papers	citations	23	40
		h-index	g-index

76	76	76	2752
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149
2	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	1.5	148
3	Mechanism of transmembrane signaling by sensor histidine kinases. Science, 2017, 356, .	6.0	132
4	Pepsi-SAXS: an adaptive method for rapid and accurate computation of small-angle X-ray scattering profiles. Acta Crystallographica Section D: Structural Biology, 2017, 73, 449-464.	1.1	99
5	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
6	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	1.5	87
7	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution. PLoS Computational Biology, 2020, 16, e1007870.	1.5	76
8	Protein model quality assessment using 3D oriented convolutional neural networks. Bioinformatics, 2019, 35, 3313-3319.	1.8	75
9	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	1.5	73
10	Deep convolutional networks for quality assessment of protein folds. Bioinformatics, 2018, 34, 4046-4053.	1.8	69
11	Smooth orientation-dependent scoring function for coarse-grained protein quality assessment. Bioinformatics, 2019, 35, 2801-2808.	1.8	54
12	Water Molecules and Hydrogen-Bonded Networks in Bacteriorhodopsinâ€"Molecular Dynamics Simulations of the Ground State and the M-Intermediate. Biophysical Journal, 2005, 88, 3252-3261.	0.2	51
13	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
14	NOLB: Nonlinear Rigid Block Normal-Mode Analysis Method. Journal of Chemical Theory and Computation, 2017, 13, 2123-2134.	2.3	50
15	Unique DC-SIGN Clustering Activity of a Small Glycomimetic: A Lesson for Ligand Design. ACS Chemical Biology, 2014, 9, 1377-1385.	1.6	47
16	Spherical polar Fourier assembly of protein complexes with arbitrary point group symmetry. Journal of Applied Crystallography, 2016, 49, 158-167.	1.9	42
17	X-ray structure of a CDP-alcohol phosphatidyltransferase membrane enzyme and insights into its catalytic mechanism. Nature Communications, 2014, 5, 4169.	5.8	39
18	Dynamical Heterogeneity of Specific Amino Acids in Bacteriorhodopsin. Journal of Molecular Biology, 2008, 380, 581-591.	2.0	35

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19	Active State of Sensory Rhodopsin II: Structural Determinants for Signal Transfer and Proton Pumping. Journal of Molecular Biology, 2011, 412, 591-600.	2.0	31
20	Protein sequenceâ€toâ€structure learning: Is this the end(â€toâ€end revolution)?. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1770-1786.	1.5	30
21	A comparison of neighbor search algorithms for large rigid molecules. Journal of Computational Chemistry, 2011, 32, 2865-2877.	1.5	28
22	Interactive quantum chemistry: A divideâ€andâ€conquer ASEDâ€MO method. Journal of Computational Chemistry, 2012, 33, 779-790.	1.5	27
23	Assessment of chemicalâ€crosslinkâ€assisted protein structure modeling in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1283-1297.	1.5	27
24	VoroCNN: deep convolutional neural network built on 3D Voronoi tessellation of protein structures. Bioinformatics, 2021, 37, 2332-2339.	1.8	27
25	Principal Component Analysis of Lipid Molecule Conformational Changes in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 1019-1028.	2.3	26
26	Practical modeling of molecular systems with symmetries. Journal of Computational Chemistry, 2010, 31, 1799-1814.	1.5	24
27	New Insights on Signal Propagation by Sensory Rhodopsin II/Transducer Complex. Scientific Reports, 2017, 7, 41811.	1.6	24
28	Convex-PL: a novel knowledge-based potential for protein-ligand interactions deduced from structural databases using convex optimization. Journal of Computer-Aided Molecular Design, 2017, 31, 943-958.	1.3	24
29	Small angle Xâ€ray scatteringâ€assisted protein structure prediction in CASP13 and emergence of solution structure differences. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1298-1314.	1.5	24
30	Rapid determination of RMSDs corresponding to macromolecular rigid body motions. Journal of Computational Chemistry, 2014, 35, 950-956.	1.5	20
31	DockTrina: Docking triangular protein trimers. Proteins: Structure, Function and Bioinformatics, 2014, 82, 34-44.	1.5	20
32	Interactive physically-based structural modeling of hydrocarbon systems. Journal of Computational Physics, 2012, 231, 2581-2598.	1.9	19
33	Two Distinct States of the HAMP Domain from Sensory Rhodopsin Transducer Observed in Unbiased Molecular Dynamics Simulations. PLoS ONE, 2013, 8, e66917.	1.1	19
34	Analytical symmetry detection in protein assemblies. I. Cyclic symmetries. Journal of Structural Biology, 2018, 203, 142-148.	1.3	19
35	PEPSI-Dock: a detailed data-driven proteinâ€“protein interaction potential accelerated by polar Fourier correlation. Bioinformatics, 2016, 32, i693-i701.	1.8	17
36	RapidRMSD: rapid determination of RMSDs corresponding to motions of flexible molecules. Bioinformatics, 2018, 34, 2757-2765.	1.8	17

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37	Analytical symmetry detection in protein assemblies. II. Dihedral and cubic symmetries. Journal of Structural Biology, 2018, 203, 185-194.	1.3	16
38	KORP-PL: a coarse-grained knowledge-based scoring function for proteinâ€“ligand interactions. Bioinformatics, 2021, 37, 943-950.	1.8	16
39	KAP1 is an antiparallel dimer with a functional asymmetry. Life Science Alliance, 2019, 2, e201900349.	1.3	16
40	Docking of small molecules to farnesoid X receptors using AutoDock Vina with the Convex-PL potential: lessons learned from D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 151-162.	1.3	15
41	Knowledge of Native Proteinâ€“Protein Interfaces Is Sufficient To Construct Predictive Models for the Selection of Binding Candidates. Journal of Chemical Information and Modeling, 2015, 55, 2242-2255.	2.5	14
42	Knodle: A Support Vector Machines-Based Automatic Perception of Organic Molecules from 3D Coordinates. Journal of Chemical Information and Modeling, 2016, 56, 1410-1419.	2.5	14
43	Role of the HAMP Domain Region of Sensory Rhodopsin Transducers in Signal Transduction. Biochemistry, 2011, 50, 574-580.	1.2	13
44	Hydroxylation of Antitubercular Drug Candidate, SQ109, by Mycobacterial Cytochrome P450. International Journal of Molecular Sciences, 2020, 21, 7683.	1.8	12
45	Predicting binding poses and affinities for protein - ligand complexes in the 2015 D3R Grand Challenge using a physical model with a statistical parameter estimation. Journal of Computer-Aided Molecular Design, 2016, 30, 791-804.	1.3	11
46	Spherical convolutions on molecular graphs for protein model quality assessment. Machine Learning: Science and Technology, 2021, 2, 045005.	2.4	11
47	Ground state structure of D75N mutant of sensory rhodopsin II in complex with its cognate transducer. Journal of Photochemistry and Photobiology B: Biology, 2013, 123, 55-58.	1.7	10
48	Interdomain Flexibility within NADPH Oxidase Suggested by SANS Using LMNG Stealth Carrier. Biophysical Journal, 2020, 119, 605-618.	0.2	9
49	Blockâ€adaptive quantum mechanics: An adaptive divideâ€andâ€conquer approach to interactive quantum chemistry. Journal of Computational Chemistry, 2013, 34, 492-504.	1.5	8
50	Predicting Binding Poses and Affinities in the CSAR 2013â€“2014 Docking Exercises Using the Knowledge-Based Convex-PL Potential. Journal of Chemical Information and Modeling, 2016, 56, 1053-1062.	2.5	8
51	DeepSymmetry: using 3D convolutional networks for identification of tandem repeats and internal symmetries in protein structures. Bioinformatics, 2019, 35, 5113-5120.	1.8	8
52	HermiteFit: fast-fitting atomic structures into a low-resolution density map using three-dimensional orthogonal Hermite functions. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2069-2084.	2.5	7
53	Eurecon: Equidistant uniform rigid-body ensemble constructor. Journal of Molecular Graphics and Modelling, 2018, 80, 313-319.	1.3	7
54	AnAnaS: Software for Analytical Analysis of Symmetries in Protein Structures. Methods in Molecular Biology, 2020, 2165, 245-257.	0.4	7

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55	Docking rigid macrocycles using Convex-PL, AutoDock Vina, and RDKit in the D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 191-200.	1.3	6
56	Predicting Protein Functional Motions: an Old Recipe with a New Twist. Biophysical Journal, 2020, 118, 2513-2525.	0.2	5
57	Fast construction of assembly trees for molecular graphs. Journal of Computational Chemistry, 2011, 32, 1589-1598.	1.5	4
58	HOPMA: Boosting Protein Functional Dynamics with Colored Contact Maps. Journal of Physical Chemistry B, 2021, 125, 2577-2588.	1.2	4
59	A novel fast Fourier transform accelerated off-grid exhaustive search method for cryo-electron microscopy fitting. Journal of Applied Crystallography, 2017, 50, 1036-1047.	1.9	2
60	Modeling and minimizing CAPRI round 30 symmetrical protein complexes from CASPâ€11 structural models. Proteins: Structure, Function and Bioinformatics, 2017, 85, 463-469.	1.5	2
61	A novel dimerization interface of cyclic nucleotide binding domain, which is disrupted in presence of cAMP: implications for CNG channels gating. Journal of Molecular Modeling, 2012, 18, 4053-4060.	0.8	1
62	Changes in the level of poly(Phe) synthesis in Escherichia coli ribosomes containing mutants of L4 ribosomal protein from Thermus thermophilus can be explained by structural changes in the peptidyltransferase center: a molecular dynamics simulation analysis. European Biophysics Journal, 2006, 35, 675-683.	1.2	0
63	Controlledâ€advancement rigidâ€body optimization of nanosystems. Journal of Computational Chemistry, 2019, 40, 2391-2399.	1.5	0
64	Title is missing!. , 2020, 16, e1007870.		0
65	Title is missing!. , 2020, 16, e1007870.		0
66	Title is missing!. , 2020, 16, e1007870.		0
67	Title is missing!. , 2020, 16, e1007870.		0