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	KORP-PL: a coarse-grained knowledge-based scoring function for proteinâ€“ligand interactions. Bioinformatics, 2021, 37, 943-950.	1.8	16
2	VoroCNN: deep convolutional neural network built on 3D Voronoi tessellation of protein structures. Bioinformatics, 2021, 37, 2332-2339.	1.8	27
3	HOPMA: Boosting Protein Functional Dynamics with Colored Contact Maps. Journal of Physical Chemistry B, 2021, 125, 2577-2588.	1.2	4
4	Spherical convolutions on molecular graphs for protein model quality assessment. Machine Learning: Science and Technology, 2021, 2, 045005.	2.4	11
5	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
6	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
7	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
8	Interdomain Flexibility within NADPH Oxidase Suggested by SANS Using LMNG Stealth Carrier. Biophysical Journal, 2020, 119, 605-618.	0.2	9
9	Hydroxylation of Antitubercular Drug Candidate, SQ109, by Mycobacterial Cytochrome P450. International Journal of Molecular Sciences, 2020, 21, 7683.	1.8	12
10	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
11	Predicting Protein Functional Motions: an Old Recipe with a New Twist. Biophysical Journal, 2020, 118, 2513-2525.	0.2	5
12	AnAnaS: Software for Analytical Analysis of Symmetries in Protein Structures. Methods in Molecular Biology, 2020, 2165, 245-257.	0.4	7
13	Title is missing!. , 2020, 16, e1007870.		0
14	Title is missing!. , 2020, 16, e1007870.		0
15	Title is missing!. , 2020, 16, e1007870.		0
16	Title is missing!. , 2020, 16, e1007870.		0
17	Controlledâ€advancement rigidâ€body optimization of nanosystems. Journal of Computational Chemistry, 2019, 40, 2391-2399.	1.5	0
18	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

#	Article	IF	Citations
19	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
20	Assessment of chemicalâ€crosslinkâ€assisted protein structure modeling in CASP13. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1283-1297.	1.5	27
21	DeepSymmetry: using 3D convolutional networks for identification of tandem repeats and internal symmetries in protein structures. Bioinformatics, 2019, 35, 5113-5120.	1.8	8
22	Protein model quality assessment using 3D oriented convolutional neural networks. Bioinformatics, 2019, 35, 3313-3319.	1.8	75
23	Smooth orientation-dependent scoring function for coarse-grained protein quality assessment. Bioinformatics, 2019, 35, 2801-2808.	1.8	54
24	KAP1 is an antiparallel dimer with a functional asymmetry. Life Science Alliance, 2019, 2, e201900349.	1.3	16
25	Eurecon: Equidistant uniform rigid-body ensemble constructor. Journal of Molecular Graphics and Modelling, 2018, 80, 313-319.	1.3	7
26	Analytical symmetry detection in protein assemblies. I. Cyclic symmetries. Journal of Structural Biology, 2018, 203, 142-148.	1.3	19
27	RapidRMSD: rapid determination of RMSDs corresponding to motions of flexible molecules. Bioinformatics, 2018, 34, 2757-2765.	1.8	17
28	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
29	Analytical symmetry detection in protein assemblies. II. Dihedral and cubic symmetries. Journal of Structural Biology, 2018, 203, 185-194.	1.3	16
30	Deep convolutional networks for quality assessment of protein folds. Bioinformatics, 2018, 34, 4046-4053.	1.8	69
31	New Insights on Signal Propagation by Sensory Rhodopsin II/Transducer Complex. Scientific Reports, 2017, 7, 41811.	1.6	24
32	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
33	Mechanism of transmembrane signaling by sensor histidine kinases. Science, 2017, 356, .	6.0	132
34	NOLB: Nonlinear Rigid Block Normal-Mode Analysis Method. Journal of Chemical Theory and Computation, 2017, 13, 2123-2134.	2.3	50
35	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
36	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

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37	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
38	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
39	Spherical polar Fourier assembly of protein complexes with arbitrary point group symmetry. Journal of Applied Crystallography, 2016, 49, 158-167.	1.9	42
40	PEPSI-Dock: a detailed data-driven proteinâ€“protein interaction potential accelerated by polar Fourier correlation. Bioinformatics, 2016, 32, i693-i701.	1.8	17
41	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
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	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
44	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
45	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
46	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	1.5	50
47	Unique DC-SIGN Clustering Activity of a Small Glycomimetic: A Lesson for Ligand Design. ACS Chemical Biology, 2014, 9, 1377-1385.	1.6	47
48	Rapid determination of RMSDs corresponding to macromolecular rigid body motions. Journal of Computational Chemistry, 2014, 35, 950-956.	1.5	20
49	X-ray structure of a CDP-alcohol phosphatidyltransferase membrane enzyme and insights into its catalytic mechanism. Nature Communications, 2014, 5, 4169.	5.8	39
50	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149
51	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
52	DockTrina: Docking triangular protein trimers. Proteins: Structure, Function and Bioinformatics, 2014, 82, 34-44.	1.5	20
53	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
54	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

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55	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
56	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
57	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
58	Interactive physically-based structural modeling of hydrocarbon systems. Journal of Computational Physics, 2012, 231, 2581-2598.	1.9	19
59	Interactive quantum chemistry: A divideâ€andâ€conquer ASEDâ€MO method. Journal of Computational Chemistry, 2012, 33, 779-790.	1.5	27
60	Role of the HAMP Domain Region of Sensory Rhodopsin Transducers in Signal Transduction. Biochemistry, 2011, 50, 574-580.	1.2	13
61	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
62	Fast construction of assembly trees for molecular graphs. Journal of Computational Chemistry, 2011, 32, 1589-1598.	1.5	4
63	A comparison of neighbor search algorithms for large rigid molecules. Journal of Computational Chemistry, 2011, 32, 2865-2877.	1.5	28
64	Practical modeling of molecular systems with symmetries. Journal of Computational Chemistry, 2010, 31, 1799-1814.	1.5	24
65	Dynamical Heterogeneity of Specific Amino Acids in Bacteriorhodopsin. Journal of Molecular Biology, 2008, 380, 581-591.	2.0	35
66	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
67	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