Sebastian Kmiecik

List of Publications by Year
in descending order

67	3,683	196777	162838
papers	citations	29 h-index	57 g-index

77	77	77	4249
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A3D 2.0 Update for the Prediction and Optimization of Protein Solubility. Methods in Molecular Biology, 2022, 2406, 65-84.	0.4	7
2	Protocols for Rational Design of Protein Solubility and Aggregation Properties Using Aggrescan3D Standalone. Methods in Molecular Biology, 2022, 2340, 17-40.	0.4	0
3	Novel Tetrazole-Based Antimicrobial Agents Targeting Clinical Bacteria Strains: Exploring the Inhibition of Staphylococcus aureus DNA Topoisomerase IV and Gyrase. International Journal of Molecular Sciences, 2022, 23, 378.	1.8	2
4	A3D database: structure-based predictions of protein aggregation for the human proteome. Bioinformatics, 2022, 38, 3121-3123.	1.8	4
5	MAPIYA contact map server for identification and visualization of molecular interactions in proteins and biological complexes. Nucleic Acids Research, 2022, 50, W474-W482.	6.5	14
6	The Effect of Conjugation of Ciprofloxacin and Moxifloxacin with Fatty Acids on Their Antibacterial and Anticancer Activity. International Journal of Molecular Sciences, 2022, 23, 6261.	1.8	9
7	Design and Synthesis of Menthol and Thymol Derived Ciprofloxacin: Influence of Structural Modifications on the Antibacterial Activity and Anticancer Properties. International Journal of Molecular Sciences, 2022, 23, 6600.	1.8	1
8	Docking of peptides to GPCRs using a combination of CABS-dock with FlexPepDock refinement. Briefings in Bioinformatics, 2021, 22, .	3.2	8
9	Molecular Dynamics Scoring of Proteinâ€“Peptide Models Derived from Coarse-Grained Docking. Molecules, 2021, 26, 3293.	1.7	7
10	Proteinâ€“Protein Docking with Large-Scale Backbone Flexibility Using Coarse-Grained Monte-Carlo Simulations. International Journal of Molecular Sciences, 2021, 22, 7341.	1.8	5
11	Phosphorylation of the conserved Câ€terminal domain of ribosomal Pâ€proteins impairs the mode of interaction with plant toxins. FEBS Letters, 2021, 595, 2221-2236.	1.3	3
12	Synthetic Transition from Thiourea-Based Compounds to Tetrazole Derivatives: Structure and Biological Evaluation of Synthesized New N-(Furan-2-ylmethyl)-1H-tetrazol-5-amine Derivatives. Molecules, 2021, 26, 323.	1.7	4
13	Flexible docking of peptides to proteins using CABSâ€dock. Protein Science, 2020, 29, 211-222.	3.1	48
14	Computational reconstruction of atomistic protein structures from coarse-grained models. Computational and Structural Biotechnology Journal, 2020, 18, 162-176.	1.9	43
15	Phosphorylation of the Nâ€terminal domain of ribosomal Pâ€stalk protein uL10 governs its association with the ribosome. FEBS Letters, 2020, 594, 3002-3019.	1.3	4
16	Isoxazole-containing 5â€² mRNA cap analogues as inhibitors of the translation initiation process. Bioorganic Chemistry, 2020, 96, 103583.	2.0	3
17	Docking interactions determine early cleavage events in insulin proteolysis by pepsin: Experiment and simulation. International Journal of Biological Macromolecules, 2020, 149, 1151-1160.	3.6	12
18	Protocols for All-Atom Reconstruction and High-Resolution Refinement of Proteinâ€“Peptide Complex Structures. Methods in Molecular Biology, 2020, 2165, 273-287.	0.4	7

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19	Protocols for Fast Simulations of Protein Structure Flexibility Using CABS-Flex and SURPASS. Methods in Molecular Biology, 2020, 2165, 337-353.	0.4	15
20	CABS-flex standalone: a simulation environment for fast modeling of protein flexibility. Bioinformatics, 2019, 35, 694-695.	1.8	79
21	Aggrescan3D (A3D) 2.0: prediction and engineering of protein solubility. Nucleic Acids Research, 2019, 47, W300-W307.	6.5	91
22	Aggrescan3D standalone package for structure-based prediction of protein aggregation properties. Bioinformatics, 2019, 35, 3834-3835.	1.8	22
23	CABS-dock standalone: a toolbox for flexible proteinâ€“peptide docking. Bioinformatics, 2019, 35, 4170-4172.	1.8	55
24	Modeling of Disordered Protein Structures Using Monte Carlo Simulations and Knowledge-Based Statistical Force Fields. International Journal of Molecular Sciences, 2019, 20, 606.	1.8	45
25	Protein Dynamics Simulations Using Coarse-Grained Models. Springer Series on Bio- and Neurosystems, 2019, , 61-87.	0.2	4
26	Proteinâ€“peptide docking using CABS-dock and contact information. Briefings in Bioinformatics, 2019, 20, 2299-2305.	3.2	35
27	Protein Structure Prediction Using Coarse-Grained Models. Springer Series on Bio- and Neurosystems, 2019, , 27-59.	0.2	3
28	Denatured proteins and early folding intermediates simulated in a reduced conformational space.. Acta Biochimica Polonica, 2019, 53, 131-143.	0.3	25
29	Synthesis, structural and antimicrobial studies of type II topoisomerase-targeted copper(II) complexes of 1,3-disubstituted thiourea ligands. Journal of Inorganic Biochemistry, 2018, 182, 61-70.	1.5	25
30	Proteinâ€“peptide docking: opportunities and challenges. Drug Discovery Today, 2018, 23, 1530-1537.	3.2	212
31	Modeling of Protein Structural Flexibility and Large-Scale Dynamics: Coarse-Grained Simulations and Elastic Network Models. International Journal of Molecular Sciences, 2018, 19, 3496.	1.8	60
32	CABS-flex 2.0: a web server for fast simulations of flexibility of protein structures. Nucleic Acids Research, 2018, 46, W338-W343.	6.5	249
33	Combining Structural Aggregation Propensity and Stability Predictions To Redesign Protein Solubility. Molecular Pharmaceutics, 2018, 15, 3846-3859.	2.3	45
34	Design and synthesis of novel 1H-tetrazol-5-amine based potent antimicrobial agents: DNA topoisomerase IV and gyrase affinity evaluation supported by molecular docking studies. European Journal of Medicinal Chemistry, 2018, 156, 631-640.	2.6	27
35	Kinetics and mechanical stability of the fibril state control fibril formation time of polypeptide chains: A computational study. Journal of Chemical Physics, 2018, 148, 215106.	1.2	21
36	Highly Flexible Protein-Peptide Docking Using CABS-Dock. Methods in Molecular Biology, 2017, 1561, 69-94.	0.4	33

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37	One-Dimensional Structural Properties of Proteins in the Coarse-Grained CABS Model. Methods in Molecular Biology, 2017, 1484, 83-113.	0.4	8
38	Modeling EphB4-EphrinB2 proteinâ€“protein interaction using flexible docking of a short linear motif. BioMedical Engineering OnLine, 2017, 16, 71.	1.3	17
39	A protocol for CABS-dock proteinâ€“peptide docking driven by side-chain contact information. BioMedical Engineering OnLine, 2017, 16, 73.	1.3	9
40	Protein-peptide molecular docking with large-scale conformational changes: the p53-MDM2 interaction. Scientific Reports, 2016, 6, 37532.	1.6	44
41	5-HT 2 receptor affinity, docking studies and pharmacological evaluation of a series of 1,3-disubstituted thiourea derivatives. European Journal of Medicinal Chemistry, 2016, 116, 173-186.	2.6	23
42	Coarse-Grained Simulations of Membrane Insertion and Folding of Small Helical Proteins Using the CABS Model. Journal of Chemical Information and Modeling, 2016, 56, 2207-2215.	2.5	17
43	Coarse-Grained Protein Models and Their Applications. Chemical Reviews, 2016, 116, 7898-7936.	23.0	721
44	Protein-Peptide Docking with High Conformational Flexibility using CABS-dock Web Tool. Biophysical Journal, 2016, 110, 543a.	0.2	1
45	Modeling of proteinâ€“peptide interactions using the CABS-dock web server for binding site search and flexible docking. Methods, 2016, 93, 72-83.	1.9	137
46	CABS-dock web server for the flexible docking of peptides to proteins without prior knowledge of the binding site. Nucleic Acids Research, 2015, 43, W419-W424.	6.5	331
47	AGGRESCAN3D (A3D): server for prediction of aggregation properties of protein structures. Nucleic Acids Research, 2015, 43, W306-W313.	6.5	201
48	CABS-flex predictions of protein flexibility compared with NMR ensembles. Bioinformatics, 2014, 30, 2150-2154.	1.8	75
49	Coarse-Grained Protein Models in Structure Prediction. Springer Series in Bio-/neuroinformatics, 2014, , 25-53.	0.1	1
50	Coarse-Grained Modeling of Protein Dynamics. Springer Series in Bio-/neuroinformatics, 2014, , 55-79.	0.1	8
51	Mechanism of Folding and Binding of an Intrinsically Disordered Protein As Revealed by ab Initio Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2224-2231.	2.3	41
52	Structure Prediction of the Second Extracellular Loop in G-Protein-Coupled Receptors. Biophysical Journal, 2014, 106, 2408-2416.	0.2	30
53	Protocols for Efficient Simulations of Long-Time Protein Dynamics Using Coarse-Grained CABS Model. Methods in Molecular Biology, 2014, 1137, 235-250.	0.4	13
54	Consistent View of Protein Fluctuations from All-Atom Molecular Dynamics and Coarse-Grained Dynamics with Knowledge-Based Force-Field. Journal of Chemical Theory and Computation, 2013, 9, 119-125.	2.3	85

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55	Combining Coarse-Grained Protein Models with Replica-Exchange All-Atom Molecular Dynamics. International Journal of Molecular Sciences, 2013, 14, 9893-9905.	1.8	22
56	CABS-flex: server for fast simulation of protein structure fluctuations. Nucleic Acids Research, 2013, 41, W427-W431.	6.5	132
57	CABS-fold: server for the de novo and consensus-based prediction of protein structure. Nucleic Acids Research, 2013, 41, W406-W411.	6.5	86
58	From Coarse-Grained to Atomic-Level Characterization of Protein Dynamics: Transition State for the Folding of B Domain of Protein A. Journal of Physical Chemistry B, 2012, 116, 7026-7032.	1.2	31
59	Optimization of protein models. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 479-493.	6.2	32
60	Simulation of Chaperonin Effect on Protein Folding: A Shift from Nucleationâ€“Condensation to Framework Mechanism. Journal of the American Chemical Society, 2011, 133, 10283-10289.	6.6	40
61	Multiscale Approach to Protein Folding Dynamics. , 2011, , 281-293.		11
62	Folding Pathway of the B1 Domain of Protein G Explored by Multiscale Modeling. Biophysical Journal, 2008, 94, 726-736.	0.2	96
63	Characterization of protein-folding pathways by reduced-space modeling. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 12330-12335.	3.3	87
64	Folding pathway of the B1 domain of protein G explored by a multiscale modeling. Nature Precedings, 2007, , .	0.1	0
65	Backbone building from quadrilaterals: A fast and accurate algorithm for protein backbone reconstruction from alpha carbon coordinates. Journal of Computational Chemistry, 2007, 28, 1593-1597.	1.5	102
66	Towards the high-resolution protein structure prediction. Fast refinement of reduced models with all-atom force field. BMC Structural Biology, 2007, 7, 43.	2.3	45
67	Denatured proteins and early folding intermediates simulated in a reduced conformational space. Acta Biochimica Polonica, 2006, 53, 131-44.	0.3	10