Jens KrÃ¼ger

List of Publications by Year
in descending order

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50	953	516710 16	477307 29
papers	citations	h-index	g-index

53	53	53	1507
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	APL@Voro: A Voronoi-Based Membrane Analysis Tool for GROMACS Trajectories. Journal of Chemical Information and Modeling, 2013, 53, 2908-2925.	5.4	100
2	Activation of lymphoma-associated MyD88 mutations via allostery-induced TIR-domain oligomerization. Blood, 2014, 124, 3896-3904.	1.4	69
3	Structural Stability of V-Amylose Helices in Water-DMSO Mixtures Analyzed by Molecular Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 2919-2928.	5.3	63
4	The MoSGrid Science Gateway â€“ A Complete Solution for Molecular Simulations. Journal of Chemical Theory and Computation, 2014, 10, 2232-2245.	5.3	58
5	TPC2 polymorphisms associated with a hair pigmentation phenotype in humans result in gain of channel function by independent mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E8595-E8602.	7.1	55
6	Regulation of Hyperpolarization-activated Cyclic Nucleotide-gated (HCN) Channel Activity by cCMP. Journal of Biological Chemistry, 2012, 287, 26506-26512.	3.4	51
7	ORF8a of SARS-CoV forms an ion channel: Experiments and molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 572-579.	2.6	50
8	CELLmicrocosmos 2.2 MembraneEditor: A Modular Interactive Shape-Based Software Approach To Solve Heterogeneous Membrane Packing Problems. Journal of Chemical Information and Modeling, 2011, 51, 1165-1182.	5.4	49
9	Assembly of Viral Membrane Proteins. Journal of Chemical Theory and Computation, 2009, 5, 2503-2513.	5.3	43
10	Iridium-Catalyzed H/D Exchange. European Journal of Organic Chemistry, 2005, 2005, 1402-1408.	2.4	40
11	A Single Sign-On Infrastructure for Science Gateways on a Use Case for Structural Bioinformatics. Journal of Grid Computing, 2012, 10, 769-790.	3.9	39
12	Exploring the conformational space of Vpu from HIVâ€1: A versatile adaptable protein. Journal of Computational Chemistry, 2008, 29, 2416-2424.	3.3	35
13	Standardsâ€based metadata management for molecular simulations. Concurrency Computation Practice and Experience, 2014, 26, 1744-1759.	2.2	26
14	Chapter 2 Viral Channel-Forming Proteins. International Review of Cell and Molecular Biology, 2009, 275, 35-63.	3.2	25
15	Genome-wide Association and Meta-analysis of Age at Onset in Parkinson Disease. Neurology, 2022, 99, .	1.1	25
16	DNA-binding proteins from marine bacteria expand the known sequence diversity of TALE-like repeats. Nucleic Acids Research, 2015, 43, gkv1053.	14.5	23
17	Enforcing SLAs in Scientific Clouds. , 2010, , .		21
18	Quantum chemical metaâ€workflows in MoSGrid. Concurrency Computation Practice and Experience, 2015, 27, 344-357.	2.2	19

#	Article	IF	Citations
19	Time resolved structure analysis of growing Î²-amyloid fibers. Journal of Structural Biology, 2007, 159, 71-81.	2.8	13
20	de.NBI Cloud federation through ELIXIR AAI. F1000Research, 2019, 8, 842.	1.6	13
21	Using Science Gateways for Bridging the Differences between Research Infrastructures. Journal of Grid Computing, 2016, 14, 545-557.	3.9	12
22	Portals and Web-Based Resources for Virtual Screening. Current Drug Targets, 2016, 17, 1649-1660.	2.1	12
23	Structural implications of mutations assessed by molecular dynamics: Vpu1â€“32 from HIV-1. European Biophysics Journal, 2010, 39, 1069-1077.	2.2	11
24	Managing Complexity in Distributed Data Life Cycles Enhancing Scientific Discovery. , 2015, , .		10
25	ballaxy: web services for structural bioinformatics. Bioinformatics, 2015, 31, 121-122.	4.1	10
26	Performance Studies on Distributed Virtual Screening. BioMed Research International, 2014, 2014, 1-7.	1.9	8
27	Gathering requirements for advancing simulations in HPC infrastructures via science gateways. Future Generation Computer Systems, 2018, 82, 544-554.	7.5	7
28	Performance and scaling behavior of bioinformatic applications in virtualization environments to create awareness for the efficient use of compute resources. PLoS Computational Biology, 2021, 17, e1009244.	3.2	7
29	Meta-Metaworkflows for Combining Quantum Chemistry and Molecular Dynamics in the MoSGrid Science Gateway. , 2014, , .		6
30	Molecular dynamics simulations and conductance studies of the interaction of VP1 N-terminus from Polio virus and gp41 fusion peptide from HIV-1 with lipid membranes. Molecular Membrane Biology, 2012, 29, 9-25.	2.0	5
31	Reproducible Scientific Workflows for High Performance and Cloud Computing. , 2019, , .		5
32	BOOTABLE: Bioinformatics benchmark tool suite for applications and hardware. Future Generation Computer Systems, 2020, 102, 1016-1026.	7.5	5
33	Cost-Aware and SLO-Fulfilling Software as a Service. Journal of Grid Computing, 2012, 10, 553-577.	3.9	4
34	User-friendly metaworkflows in quantum chemistry. , 2013, , .		4
35	Molecular Simulation Grid (MosGrid): A Science Gateway Tailored to the Molecular Simulation Community. , 2014, , 151-165.		4
36	Metadata Management in the MoSGrid Science Gateway - Evaluation and the Expansion of Quantum Chemistry Support. Journal of Grid Computing, 2017, 15, 41-53.	3.9	4

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37	A Science Gateway Getting Ready for Serving the International Molecular Simulation Community. , 2012, , .		4
38	Challenges and Modifications for Creating a MoSGrid Science Gateway for US and European Infrastructures. , 2015, , .		3
39	Multi-level meta-workflows: new concept for regularly occurring tasks in quantum chemistry. Journal of Cheminformatics, 2016, 8, 58.	6.1	3
40	WS-PGRADE/gUSE-Based Science Gateways in Teaching. , 2014, , 223-234.		3
41	Workflow-enhanced conformational analysis of guanidine zinc complexes via a science gateway. Studies in Health Technology and Informatics, 2012, 175, 142-51.	0.3	2
42	Expansion of Quantum Chemical Metadata for Workflows in the MoSGrid Science Gateway. , 2014, , .		1
43	Membrane simulation analysis using Voronoi tessellation. Journal of Cheminformatics, 2014, 6, O23.	6.1	1
44	Molecular simulation grid. Journal of Cheminformatics, 2011, 3, .	6.1	0
45	The GMX-Plugin for the CELLmicrocosmos MembraneEditor. Journal of Cheminformatics, 2012, 4, .	6.1	0
46	Integration of eSBMTools into the MoSGrid Portal Using the gUSE Technology. , 2014, , .		0
47	Multi-layer Meta-metaworkflows for the Evaluation of Solvent and Dispersion Effects in Transition Metal Systems Using the MoSGrid Science Gateways. , 2015, , .		0
48	Science gateways - leveraging modeling and simulations in HPC infrastructures via increased usability. , 2015, , .		0
49	BOOTABLE: Bioinformatics Benchmark Tool Suite. , 2019, , .		0
50	Maintaining a Science Gateway - Lessons Learned from MoSGrid. , 2017, , .		0