Vytautas Gapsys

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5631627/publications.pdf

Version: 2024-02-01

50 papers	2,302 citations	257450 24 h-index	233421 45 g-index
62 all docs	62 docs citations	62 times ranked	2520 citing authors

#	Article	IF	Citations
1	<scp>Preâ€exascale HPC</scp> approaches for molecular dynamics simulations. Covidâ€19 research: A use case. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	6
2	Pre-Exascale Computing of Proteinâ€“Ligand Binding Free Energies with Open Source Software for Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1172-1177.	5.4	22
3	GROMACS in the Cloud: A Global Supercomputer to Speed Up Alchemical Drug Design. Journal of Chemical Information and Modeling, 2022, 62, 1691-1711.	5.4	37
4	Repositioning Food and Drug Administration-Approved Drugs for Inhibiting Biliverdin IXÎ² Reductase B as a Novel Thrombocytopenia Therapeutic Target. Journal of Medicinal Chemistry, 2022, 65, 2548-2557.	6.4	1
5	A litmus test for classifying recognition mechanisms of transiently binding proteins. Nature Communications, 2022, 13, .	12.8	13
6	Non-equilibrium approach for binding free energies in cyclodextrins in SAMPL7: force fields and software. Journal of Computer-Aided Molecular Design, 2021, 35, 49-61.	2.9	23
7	One Plus One Makes Three: Triangular Coupling of Correlated Amino Acid Mutations. Journal of Physical Chemistry Letters, 2021, 12, 3195-3201.	4.6	4
8	Challenges Encountered Applying Equilibrium and Nonequilibrium Binding Free Energy Calculations. Journal of Physical Chemistry B, 2021, 125, 4241-4261.	2.6	33
9	Accurate absolute free energies for ligandâ€“protein binding based on non-equilibrium approaches. Communications Chemistry, 2021, 4, .	4.5	49
10	Alchemical absolute proteinâ€“ligand binding free energies for drug design. Chemical Science, 2021, 12, 13958-13971.	7.4	48
11	Comment on â€œDeficiencies in Molecular Dynamics Simulation-Based Prediction of Protein-DNA Binding Free Energy Landscapesâ€. Journal of Physical Chemistry B, 2020, 124, 1115-1123.	2.6	4
12	Large scale relative protein ligand binding affinities using non-equilibrium alchemy. Chemical Science, 2020, 11, 1140-1152.	7.4	147
13	Polycationâ€“Anionic Lipid Membrane Interactions. Langmuir, 2020, 36, 12435-12450.	3.5	27
14	Non-active site mutants of HIV-1 protease influence resistance and sensitisation towards protease inhibitors. Retrovirology, 2020, 17, 13.	2.0	12
15	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	2.9	86
16	On the importance of statistics in molecular simulations for thermodynamics, kinetics and simulation box size. ELife, 2020, 9, .	6.0	34
17	Predicting Kinase Inhibitor Resistance: Physics-Based and Data-Driven Approaches. ACS Central Science, 2019, 5, 1468-1474.	11.3	40
18	Performance evaluation of molecular docking and free energy calculations protocols using the D3R Grand Challenge 4 dataset. Journal of Computer-Aided Molecular Design, 2019, 33, 1031-1043.	2.9	12

#	Article	IF	Citations
19	Pyruvate carboxylase deficiency type A and type C: Characterization of five novel pathogenic variants inPCand analysis of the genotypeâ€“phenotype correlation. Human Mutation, 2019, 40, 816-827.	2.5	16
20	Accurate Calculation of Free Energy Changes upon Amino Acid Mutation. Methods in Molecular Biology, 2019, 1851, 19-47.	0.9	32
21	Comment on 'Valid molecular dynamics simulations of human hemoglobin require a surprisingly large box size'. ELife, 2019, 8, .	6.0	35
22	Utilizing dipole-dipole cross-correlated relaxation for the measurement of angles between pairs of opposing CÎ±HÎ±-CÎ±HÎ± bonds in anti-parallel Î²-sheets. Methods, 2018, 138-139, 85-92.	3.8	8
23	A Unified Framework for Alchemical Mutations in Proteins, DNA and Ligands. Biophysical Journal, 2018, 114, 674a.	0.5	0
24	Accurate Estimation of Ligand Binding Affinity Changes upon Protein Mutation. ACS Central Science, 2018, 4, 1708-1718.	11.3	82
25	Consistent Prediction of Mutation Effect on Drug Binding in HIV-1 Protease Using Alchemical Calculations. Journal of Chemical Theory and Computation, 2018, 14, 3397-3408.	5.3	24
26	pmx Webserver: A User Friendly Interface for Alchemistry. Journal of Chemical Information and Modeling, 2017, 57, 109-114.	5.4	50
27	Resolving the Atomistic Modes of Anle138b Inhibitory Action on Peptide Oligomer Formation. ACS Chemical Neuroscience, 2017, 8, 2791-2808.	3.5	26
28	Alchemical Free Energy Calculations for Nucleotide Mutations in Proteinâ€“DNA Complexes. Journal of Chemical Theory and Computation, 2017, 13, 6275-6289.	5.3	42
29	Accurate and Rigorous Prediction of the Changes in Protein Free Energies in a Largeâ€Scale Mutation Scan. Angewandte Chemie, 2016, 128, 7490-7494.	2.0	13
30	Global and Local Conformational Heterogeniety Governs the Pre-Nucleation Phase in Amyloidogenic Self-Assembly. Biophysical Journal, 2016, 110, 402a.	0.5	0
31	Insights into the molecular basis for substrate binding and specificity of the wild-type L-arginine/agmatine antiporter AdiC. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10358-10363.	7.1	82
32	An Atomistic View of Amyloidogenic Self-assembly: Structure and Dynamics of Heterogeneous Conformational States in the Pre-nucleation Phase. Scientific Reports, 2016, 6, 33156.	3.3	25
33	Accurate and Rigorous Prediction of the Changes in Protein Free Energies in a Largeâ€Scale Mutation Scan. Angewandte Chemie - International Edition, 2016, 55, 7364-7368.	13.8	111
34	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. Biophysical Journal, 2016, 110, 358a.	0.5	1
35	Insights from the First Principles Based Large Scale Protein Thermostability Calculations. Biophysical Journal, 2016, 110, 368a.	0.5	3
36	Structural Ensembles of Intrinsically Disordered Proteins using Molecular Dynamics Simulation. Biophysical Journal, 2015, 108, 14a.	0.5	1

#	Article	IF	Citations
37	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field: A Comparison to Experiment. Journal of Chemical Theory and Computation, 2015, 11, 5513-5524.	5.3	368
38	Improved validation of IDP ensembles by one-bond CÎ±â€“HÎ± scalar couplings. Journal of Biomolecular NMR, 2015, 63, 299-307.	2.8	4
39	pmx: Automated protein structure and topology generation for alchemical perturbations. Journal of Computational Chemistry, 2015, 36, 348-354.	3.3	199
40	Calculation of Binding Free Energies. Methods in Molecular Biology, 2015, 1215, 173-209.	0.9	95
41	Structural Ensembles of Intrinsically Disordered Proteins Depend Strongly on Force Field. Biophysical Journal, 2014, 106, 271a.	0.5	2
42	Computational Thrombin Inhibitor Optimization. Biophysical Journal, 2014, 106, 262a-263a.	0.5	0
43	Phosphorylation Drives a Dynamic Switch in Serine/Arginine-Rich Proteins. Structure, 2013, 21, 2162-2174.	3.3	101
44	Computational analysis of local membrane properties. Journal of Computer-Aided Molecular Design, 2013, 27, 845-858.	2.9	143
45	Optimal Superpositioning of Flexible Molecule Ensembles. Biophysical Journal, 2013, 104, 196-207.	0.5	25
46	Driving Forces and Structural Determinants of Steric Zipper Peptide Oligomer Formation Elucidated by Atomistic Simulations. Journal of Molecular Biology, 2012, 421, 390-416.	4.2	64
47	New Soft-Core Potential Function for Molecular Dynamics Based Alchemical Free Energy Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2373-2382.	5.3	92
48	Non-Equilibrium Free Energy Calculations for Ligand Optimization. Biophysical Journal, 2012, 102, 40a.	0.5	0
49	Lipid Protein Interactions and Dynamical Properties of VDAC 1 channel. Biophysical Journal, 2011, 100, 147a.	0.5	0
50	Mapping the Conformational Dynamics and Pathways of Spontaneous Steric Zipper Peptide Oligomerization. PLoS ONE, 2011, 6, e19129.	2.5	45