Samuel Genheden

List of Publications by Year
in descending order

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52 papers	5,321 citations	230014 27 h-index	214428 50 g-index
65 all docs	65 docs citations	65 times ranked	7415 citing authors

#	Article	IF	Citations
1	Fast prediction of distances between synthetic routes with deep learning. Machine Learning: Science and Technology, 2022, 3, 015018.	2.4	4
2	AI for drug design: From explicit rules to deep learning. Artificial Intelligence in the Life Sciences, 2022, 2, 100041.	1.6	4
3	Molecular-dynamics-simulation-guided membrane engineering allows the increase of membrane fatty acid chain length in Saccharomyces cerevisiae. Scientific Reports, 2021, 11, 17333.	1.6	3
4	Clustering of Synthetic Routes Using Tree Edit Distance. Journal of Chemical Information and Modeling, 2021, 61, 3899-3907.	2.5	8
5	AiZynthFinder: a fast, robust and flexible open-source software for retrosynthetic planning. Journal of Cheminformatics, 2020, 12, 70.	2.8	132
6	Mechanism of Trehalose-Induced Protein Stabilization from Neutron Scattering and Modeling. Journal of Physical Chemistry B, 2019, 123, 3679-3687.	1.2	28
7	AI-assisted synthesis prediction. Drug Discovery Today: Technologies, 2019, 32-33, 65-72.	4.0	29
8	Alcohols enhance the rate of acetic acid diffusion in S. cerevisiae: biophysical mechanisms and implications for acetic acid tolerance. Microbial Cell, 2018, 5, 42-55.	1.4	22
9	A Hybrid All-Atom/Coarse-Grained Approach to Problems in Chemistry and Biology. Biophysical Journal, 2017, 112, 177a.	0.2	0
10	G protein coupled receptor interactions with cholesterol deep in the membrane. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 268-281.	1.4	58
11	Can System Truncation Speed up Ligand-Binding Calculations with Periodic Free-Energy Simulations?. Journal of Chemical Information and Modeling, 2017, 57, 2865-2873.	2.5	0
12	Solvation free energies and partition coefficients with the coarse-grained and hybrid all-atom/coarse-grained MARTINI models. Journal of Computer-Aided Molecular Design, 2017, 31, 867-876.	1.3	22
13	Effect of solvent model when probing protein dynamics with molecular dynamics. Journal of Molecular Graphics and Modelling, 2017, 71, 80-87.	1.3	2
14	Sphingolipids contribute to acetic acid resistance in Zygosaccharomyces bailii. Biotechnology and Bioengineering, 2016, 113, 744-753.	1.7	54
15	All-atom/coarse-grained hybrid predictions of distribution coefficients in SAMPL5. Journal of Computer-Aided Molecular Design, 2016, 30, 969-976.	1.3	8
16	Estimation of Liposome Penetration Barriers of Drug Molecules with All-Atom and Coarse-Grained Models. Journal of Chemical Theory and Computation, 2016, 12, 4651-4661.	2.3	11
17	Predicting Partition Coefficients with a Simple All-Atom/Coarse-Grained Hybrid Model. Journal of Chemical Theory and Computation, 2016, 12, 297-304.	2.3	25
18	Coarse-grained bond and angle distributions from atomistic simulations: On the systematic parameterisation of lipid models. Journal of Molecular Graphics and Modelling, 2016, 63, 57-64.	1.3	3

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19	Binding affinities by alchemical perturbation using <scp>QM/MM</scp> with a large <scp>QM</scp> system and polarizable <scp>MM</scp> model. Journal of Computational Chemistry, 2015, 36, 2114-2124.	1.5	38
20	The MM/PBSA and MM/GBSA methods to estimate ligand-binding affinities. Expert Opinion on Drug Discovery, 2015, 10, 449-461.	2.5	2,907
21	A Simple and Transferable All-Atom/Coarse-Grained Hybrid Model to Study Membrane Processes. Journal of Chemical Theory and Computation, 2015, 11, 4749-4759.	2.3	32
22	Extensive all-atom Monte Carlo sampling and QM/MM corrections in the SAMPL4 hydration free energy challenge. Journal of Computer-Aided Molecular Design, 2014, 28, 187-200.	1.3	38
23	A Large-Scale Test of Free-Energy Simulation Estimates of Proteinâ€“Ligand Binding Affinities. Journal of Chemical Information and Modeling, 2014, 54, 2794-2806.	2.5	54
24	Conformational Entropies and Order Parameters: Convergence, Reproducibility, and Transferability. Journal of Chemical Theory and Computation, 2014, 10, 432-438.	2.3	31
25	Effect of explicit water molecules on ligand-binding affinities calculated with the MM/GBSA approach. Journal of Molecular Modeling, 2014, 20, 2273.	0.8	35
26	Free-energy perturbation and quantum mechanical study of SAMPL4 octa-acid hostâ€“guest binding energies. Journal of Computer-Aided Molecular Design, 2014, 28, 375-400.	1.3	70
27	Comparison of MM/GBSA calculations based on explicit and implicit solvent simulations. Physical Chemistry Chemical Physics, 2013, 15, 7731.	1.3	76
28	Amino Acid Oxidation of Candida antarctica Lipase B Studied by Molecular Dynamics Simulations and Site-Directed Mutagenesis. Biochemistry, 2013, 52, 1280-1289.	1.2	21
29	OF MICE AND MEN: DISSECTING THE INTERACTION BETWEEN LISTERIA MONOCYTOGENES INTERNALIN A AND E-CADHERIN. Computational and Structural Biotechnology Journal, 2013, 6, e201303022.	1.9	1
30	The Normal-Mode Entropy in the MM/GBSA Method: Effect of System Truncation, Buffer Region, and Dielectric Constant. Journal of Chemical Information and Modeling, 2012, 52, 2079-2088.	2.5	166
31	The Carbohydrate-Binding Site in Galectin-3 Is Preorganized To Recognize a Sugarlike Framework of Oxygens: Ultra-High-Resolution Structures and Water Dynamics. Biochemistry, 2012, 51, 296-306.	1.2	137
32	Are Homology Models Sufficiently Good for Free-Energy Simulations?. Journal of Chemical Information and Modeling, 2012, 52, 3013-3021.	2.5	8
33	Can the protonation state of histidine residues be determined from molecular dynamics simulations?. Computational and Theoretical Chemistry, 2012, 1000, 75-84.	1.1	30
34	Transferability of conformational dependent charges from protein simulations. International Journal of Quantum Chemistry, 2012, 112, 1768-1785.	1.0	10
35	Comparison of endâ€point continuumâ€solvation methods for the calculation of proteinâ€“ligand binding free energies. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1326-1342.	1.5	78
36	Will molecular dynamics simulations of proteins ever reach equilibrium?. Physical Chemistry Chemical Physics, 2012, 14, 8662.	1.3	85

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37	Improving the Efficiency of Proteinâ€“Ligand Binding Free-Energy Calculations by System Truncation. Journal of Chemical Theory and Computation, 2012, 8, 1449-1458.	2.3	18
38	Binding affinities in the SAMPL3 trypsin and hostâ€“guest blind tests estimated with the MM/PBSA and LIE methods. Journal of Computer-Aided Molecular Design, 2012, 26, 527-541.	1.3	46
39	A semiempirical approach to ligandâ€binding affinities: Dependence on the Hamiltonian and corrections. Journal of Computational Chemistry, 2012, 33, 1179-1189.	1.5	28
40	Binding Affinities of Factor Xa Inhibitors Estimated by Thermodynamic Integration and MM/GBSA. Journal of Chemical Information and Modeling, 2011, 51, 947-958.	2.5	72
41	Comparison of the Efficiency of the LIE and MM/GBSA Methods to Calculate Ligand-Binding Energies. Journal of Chemical Theory and Computation, 2011, 7, 3768-3778.	2.3	71
42	Accurate Predictions of Nonpolar Solvation Free Energies Require Explicit Consideration of Binding-Site Hydration. Journal of the American Chemical Society, 2011, 133, 13081-13092.	6.6	56
43	A QM/MM study of the binding of RAPTA ligands to cathepsin B. Journal of Computer-Aided Molecular Design, 2011, 25, 729-742.	1.3	36
44	MM/GBSA and LIE estimates of hostâ€“guest affinities: dependence on charges and solvation model. Journal of Computer-Aided Molecular Design, 2011, 25, 1085-1093.	1.3	24
45	A comparison of different initialization protocols to obtain statistically independent molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 187-195.	1.5	59
46	How to obtain statistically converged MM/GBSA results. Journal of Computational Chemistry, 2010, 31, 837-846.	1.5	167
47	Estimates of ligand-binding affinities supported by quantum mechanical methods. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 21-37.	2.2	21
48	Protein Flexibility and Conformational Entropy in Ligand Design Targeting the Carbohydrate Recognition Domain of Galectin-3. Journal of the American Chemical Society, 2010, 132, 14577-14589.	6.6	209
49	Nonpolar Solvation Free Energies of Proteinâ^'Ligand Complexes. Journal of Chemical Theory and Computation, 2010, 6, 3558-3568.	2.3	26
50	Starting-Condition Dependence of Order Parameters Derived from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2010, 6, 2176-2190.	2.3	38
51	An MM/3D-RISM Approach for Ligand Binding Affinities. Journal of Physical Chemistry B, 2010, 114, 8505-8516.	1.2	129
52	Conformational entropy changes upon lactose binding to the carbohydrate recognition domain of galectin-3. Journal of Biomolecular NMR, 2009, 45, 157-169.	1.6	75