Jonathan W Essex

List of Publications by Year
in descending order

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117 papers	5,608 citations	57631 44 h-index	85405 71 g-index
126 all docs	126 docs citations	126 times ranked	5582 citing authors

#	Article	IF	Citations
1	How well does molecular simulation reproduce environment-specific conformations of the intrinsically disordered peptides PLP, TP2 and ONEG?. Chemical Science, 2022, 13, 1957-1971.	3.7	7
2	Enhancing Sampling of Water Rehydration on Ligand Binding: A Comparison of Techniques. Journal of Chemical Theory and Computation, 2022, 18, 1359-1381.	2.3	22
3	Comparison of Grand Canonical and Conventional Molecular Dynamics Simulation Methods for Protein-Bound Water Networks. ACS Physical Chemistry Au, 2022, 2, 247-259.	1.9	4
4	Enhancing Ligand and Protein Sampling Using Sequential Monte Carlo. Journal of Chemical Theory and Computation, 2022, , .	2.3	5
5	Higher Affinity Antibodies Bind With Lower Hydration and Flexibility in Large Scale Simulations. Frontiers in Immunology, 2022, 13, .	2.2	1
6	Hinge disulfides in human IgG2 CD40 antibodies modulate receptor signaling by regulation of conformation and flexibility. Science Immunology, 2022, 7, .	5.6	18
7	Coarse-Grained Molecular Dynamics Simulations of Membrane Proteins: A Practical Guide. Methods in Molecular Biology, 2021, 2302, 253-273.	0.4	3
8	Water molecules at proteinâ€“drug interfaces: computational prediction and analysis methods. Chemical Society Reviews, 2021, 50, 9104-9120.	18.7	34
9	Sensitivity of Binding Free Energy Calculations to Initial Protein Crystal Structure. Journal of Chemical Theory and Computation, 2021, 17, 1806-1821.	2.3	13
10	ParaMol: A Package for Automatic Parameterization of Molecular Mechanics Force Fields. Journal of Chemical Information and Modeling, 2021, 61, 2026-2047.	2.5	22
11	Computational Methods and Tools in Antimicrobial Peptide Research. Journal of Chemical Information and Modeling, 2021, 61, 3172-3196.	2.5	51
12	Rimantadine Binds to and Inhibits the Influenza A M2 Proton Channel without Enantiomeric Specificity. Biochemistry, 2021, 60, 2471-2482.	1.2	10
13	The automated optimisation of a coarse-grained force field using free energy data. Physical Chemistry Chemical Physics, 2021, 23, 24842-24851.	1.3	3
14	Generation of Quantum Configurational Ensembles Using Approximate Potentials. Journal of Chemical Theory and Computation, 2021, 17, 7021-7042.	2.3	2
15	BRIDGE: An Open Platform for Reproducible High-Throughput Free Energy Simulations. Journal of Chemical Information and Modeling, 2020, 60, 5290-5295.	2.5	10
16	grand: A Python Module for Grand Canonical Water Sampling in OpenMM. Journal of Chemical Information and Modeling, 2020, 60, 4436-4441.	2.5	24
17	ProtoCaller: Robust Automation of Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 1917-1921.	2.5	18
18	Molecular Dynamics Simulations of Antibiotic Ceftaroline at the Allosteric Site of Penicillinâ€Binding Protein 2a (PBP2a). Israel Journal of Chemistry, 2020, 60, 754-763.	1.0	15

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19	The Role of Electrostatics in Enzymes: Do Biomolecular Force Fields Reflect Protein Electric Fields?. Journal of Chemical Information and Modeling, 2020, 60, 3131-3144.	2.5	29
20	The role of molecular simulations in understanding the mechanisms of cell-penetrating peptides. Drug Discovery Today, 2019, 24, 1821-1835.	3.2	45
21	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	6.2	110
22	Large-scale analysis of water stability in bromodomain binding pockets with grand canonical Monte Carlo. Communications Chemistry, 2018, 1, .	2.0	52
23	Prediction of the Closed Conformation and Insights into the Mechanism of the Membrane Enzyme LpxR. Biophysical Journal, 2018, 115, 1445-1456.	0.2	4
24	Ligand Binding Free Energies with Adaptive Water Networks: Two-Dimensional Grand Canonical Alchemical Perturbations. Journal of Chemical Theory and Computation, 2018, 14, 6586-6597.	2.3	32
25	Surface reconstruction amendment to the intrinsic sampling method. Journal of Chemical Physics, 2018, 149, 234705.	1.2	2
26	Evaluating Anti-CD32b F(ab) Conformation Using Molecular Dynamics and Small-Angle X-Ray Scattering. Biophysical Journal, 2018, 115, 289-299.	0.2	4
27	Unexpected finite size effects in interfacial systems: Why bigger is not always betterâ€"Increase in uncertainty of surface tension with bulk phase width. Journal of Chemical Physics, 2018, 148, 214704.	1.2	5
28	Conformation and Dynamics of Human Urotensin II and Urotensin Related Peptide in Aqueous Solution. Journal of Chemical Information and Modeling, 2017, 57, 298-310.	2.5	12
29	PyCGTOOL: Automated Generation of Coarse-Grained Molecular Dynamics Models from Atomistic Trajectories. Journal of Chemical Information and Modeling, 2017, 57, 650-656.	2.5	66
30	A Monte Carlo Resampling Approach for the Calculation of Hybrid Classical and Quantum Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 415-424.	2.3	7
31	G protein coupled receptor interactions with cholesterol deep in the membrane. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 268-281.	1.4	58
32	Replica-Exchange and Standard State Binding Free Energies with Grand Canonical Monte Carlo. Journal of Chemical Theory and Computation, 2017, 13, 6373-6381.	2.3	39
33	On the Calculation of Acyl Chain Order Parameters from Lipid Simulations. Journal of Chemical Theory and Computation, 2017, 13, 5683-5696.	2.3	92
34	CD1b-restricted GEM T cell responses are modulated byMycobacterium tuberculosismycolic acid meromycolate chains. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10956-E10964.	3.3	58
35	Reactivation of mutant p53: Constraints on mechanism highlighted by principal component analysis of the DNA binding domain. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1443-1461.	1.5	10
36	All-atom/coarse-grained hybrid predictions of distribution coefficients in SAMPL5. Journal of Computer-Aided Molecular Design, 2016, 30, 969-976.	1.3	8

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37	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	1.2	77
38	Evaluating Parametrization Protocols for Hydration Free Energy Calculations with the AMOEBA Polarizable Force Field. Journal of Chemical Theory and Computation, 2016, 12, 3871-3883.	2.3	27
39	Evaluation of solvation free energies for small molecules with the AMOEBA polarizable force field. Journal of Computational Chemistry, 2016, 37, 2749-2758.	1.5	31
40	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
41	Cholesteryl esters stabilize human CD1c conformations for recognition by self-reactive T cells. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E1266-75.	3.3	41
42	Direct Validation of the Single Step Classical to Quantum Free Energy Perturbation. Journal of Physical Chemistry B, 2015, 119, 1017-1025.	1.2	45
43	X-ray crystallographic and EPR spectroscopic analysis of HydG, a maturase in [FeFe]-hydrogenase H-cluster assembly. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 1362-1367.	3.3	97
44	Water Sites, Networks, And Free Energies with Grand Canonical Monte Carlo. Journal of the American Chemical Society, 2015, 137, 14930-14943.	6.6	98
45	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
46	A Computational Study of Vicinal Fluorination in 2,3â€Difluorobutane: Implications for Conformational Control in Alkane Chains. Chemistry - A European Journal, 2015, 21, 1682-1691.	1.7	24
47	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
48	Strategies to Calculate Water Binding Free Energies in Proteinâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2014, 54, 1623-1633.	2.5	47
49	Free Energies of Binding from Large-Scale First-Principles Quantum Mechanical Calculations: Application to Ligand Hydration Energies. Journal of Physical Chemistry B, 2013, 117, 9478-9485.	1.2	41
50	Physical properties of mixed bilayers containing lamellar and nonlamellar lipids: insights from coarse-grain molecular dynamics simulations. Faraday Discussions, 2013, 161, 249-272.	1.6	61
51	Water Network Perturbation in Ligand Binding: Adenosine A_{2A} Antagonists as a Case Study. Journal of Chemical Information and Modeling, 2013, 53, 1700-1713.	2.5	114
52	Dual-resolution molecular dynamics simulation of antimicrobials in biomembranes. Journal of the Royal Society Interface, 2011, 8, 826-841.	1.5	52
53	A Simple QM/MM Approach for Capturing Polarization Effects in Proteinâ^'Ligand Binding Free Energy Calculations. Journal of Physical Chemistry B, 2011, 115, 4911-4926.	1.2	97
54	Pocket-Space Maps To Identify Novel Binding-Site Conformations in Proteins. Journal of Chemical Information and Modeling, 2011, 51, 2666-2679.	2.5	39

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55	The ELBA Force Field for Coarse-Grain Modeling of Lipid Membranes. PLoS ONE, 2011, 6, e28637.	1.1	148
56	Prediction of proteinâ€“ligand binding affinity by free energy simulations: assumptions, pitfalls and expectations. Journal of Computer-Aided Molecular Design, 2010, 24, 639-658.	1.3	221
57	Rigorous Free Energy Calculations in Structureâ€Based Drug Design. Molecular Informatics, 2010, 29, 570-578.	1.4	71
58	Coarse-grain modelling of DMPC and DOPC lipid bilayers. Journal of Physics Condensed Matter, 2010, 22, 155106.	0.7	67
59	Permeability of drugs and hormones through a lipid bilayer: insights from dual-resolution molecular dynamics. Soft Matter, 2010, 6, 3797.	1.2	132
60	Anisotropic Elastic Network Modeling of Entire Microtubules. Biophysical Journal, 2010, 99, 2190-2199.	0.2	91
61	Ensemble Docking into Multiple Crystallographically Derived Protein Structures: An Evaluation Based on the Statistical Analysis of Enrichments. Journal of Chemical Information and Modeling, 2010, 50, 511-524.	2.5	126
62	Probing the microscopic flexibility of DNA from melting temperatures. Nature Physics, 2009, 5, 769-773.	6.5	54
63	Permeability of Small Molecules through a Lipid Bilayer: A Multiscale Simulation Study. Journal of Physical Chemistry B, 2009, 113, 12019-12029.	1.2	147
64	Study of the Conformational Dynamics of the Catalytic Loop of WT and G140A/G149A HIV-1 Integrase Core Domain Using Reversible Digitally Filtered Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 411-421.	2.3	17
65	Assessment of Nonequilibrium Free Energy Methods. Journal of Physical Chemistry B, 2009, 113, 5508-5519.	1.2	26
66	Conformational Motions of HIV-1 Protease Identified Using Reversible Digitally Filtered Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 1117-1128.	2.3	9
67	Pattern recognition based on color-coded quantum mechanical surfaces for molecular alignment. Journal of Molecular Modeling, 2008, 14, 49-57.	0.8	4
68	e-Malaria: the schools Malaria project. Concurrency Computation Practice and Experience, 2008, 20, 225-238.	1.4	2
69	Hit Identification and Binding Mode Predictions by Rigorous Free Energy Simulations. Journal of Medicinal Chemistry, 2008, 51, 6654-6664.	2.9	59
70	Prediction of Partition Coefficients by Multiscale Hybrid Atomic-Level/Coarse-Grain Simulations. Journal of Physical Chemistry B, 2008, 112, 657-660.	1.2	82
71	A Quantitative Coarse-Grain Model for Lipid Bilayers. Journal of Physical Chemistry B, 2008, 112, 802-815.	1.2	119
72	Proteinâ˜Ligand Binding Affinity by Nonequilibrium Free Energy Methods. Journal of Physical Chemistry B, 2008, 112, 14985-14992.	1.2	10

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73	Optimal Probe Length Varies for Targets with High Sequence Variation: Implications for Probe Library Design for Resequencing Highly Variable Genes. PLoS ONE, 2008, 3, e2500.	1.1	3
74	Classification of Water Molecules in Protein Binding Sites. Journal of the American Chemical Society, 2007, 129, 2577-2587.	6.6	259
75	Proteinâ^'Ligand Complexes:â€‰ Computation of the Relative Free Energy of Different Scaffolds and Binding Modes. Journal of Chemical Theory and Computation, 2007, 3, 1645-1655.	2.3	43
76	Three hydrolases and a transferase: Comparative analysis of active-site dynamics via the BioSimGrid database. Journal of Molecular Graphics and Modelling, 2007, 25, 896-902.	1.3	7
77	BioSimGrid: Grid-enabled biomolecular simulation data storage and analysis. Future Generation Computer Systems, 2006, 22, 657-664.	4.9	29
78	Protein-Ligand Binding Affinity Predictions by Implicit Solvent Simulations:Â A Tool for Lead Optimization?. Journal of Medicinal Chemistry, 2006, 49, 7427-7439.	2.9	92
79	Quality Assurance for Biomolecular Simulations. Journal of Chemical Theory and Computation, 2006, 2, 1477-1481.	2.3	17
80	A Computer-Aided Drug Discovery System for Chemistry Teaching. Journal of Chemical Information and Modeling, 2006, 46, 960-970.	2.5	10
81	Efficient Generalized Born Models for Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2006, 2, 732-739.	2.3	27
82	Thermal equivalence of DNA duplexes without calculation of melting temperature. Nature Physics, 2006, 2, 55-59.	6.5	41
83	Mechanism and structureâ€“activity relationships of norspermidine-based peptidic inhibitors of trypanothione reductase. Bioorganic and Medicinal Chemistry, 2005, 13, 4513-4526.	1.4	20
84	An analysis of the feasibility of short read sequencing. Nucleic Acids Research, 2005, 33, e171-e171.	6.5	97
85	Parametrization of Reversible Digitally Filtered Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2005, 1, 24-35.	2.3	5
86	The parameterization and validation of generalized born models using the pairwise descreening approximation. Journal of Computational Chemistry, 2004, 25, 1760-1770.	1.5	11
87	BioSimGrid: towards a worldwide repository for biomolecular simulations. Organic and Biomolecular Chemistry, 2004, 2, 3219.	1.5	42
88	Permeation of Small Molecules through a Lipid Bilayer:Â A Computer Simulation Study. Journal of Physical Chemistry B, 2004, 108, 4875-4884.	1.2	255
89	Conformational and Enantioselectivity in Hostâ^'Guest Chemistry:â€‰ The Selective Binding of Cis Amides Examined by Free Energy Calculations. Journal of Physical Chemistry B, 2004, 108, 17571-17582.	1.2	4
90	FDS: Flexible ligand and receptor docking with a continuum solvent model and soft-core energy function. Journal of Computational Chemistry, 2003, 24, 1637-1656.	1.5	94

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91	Solid-phase synthesis of a focused library of trypanothione reductase inhibitors. Tetrahedron Letters, 2003, 44, 3195-3197.	0.7	15
92	Enhanced Configurational Sampling in Binding Free-Energy Calculations. Journal of Physical Chemistry B, 2003, 107, 13711-13718.	1.2	70
93	Application of the Hilbertâ^'Huang Transform to the Analysis of Molecular Dynamics Simulations. Journal of Physical Chemistry A, 2003, 107, 4869-4876.	1.1	45
94	The Development of Replica-Exchange-Based Free-Energy Methods. Journal of Physical Chemistry B, 2003, 107, 13703-13710.	1.2	166
95	Reversible Digitally Filtered Molecular Dynamics. Journal of Physical Chemistry B, 2003, 107, 2098-2110.	1.2	13
96	Fluoride-Selective Binding in a New Deep Cavity Calix[4]pyrrole:â€‰ Experiment and Theory. Journal of the American Chemical Society, 2002, 124, 8644-8652.	6.6	119
97	Molecular dynamics simulation of the hydrocarbon region of a biomembrane using a reduced representation model. Journal of Computational Chemistry, 2001, 22, 1622-1633.	1.5	52
98	The configurational dependence of binding free energies: a Poisson-Boltzmann study of Neuraminidase inhibitors. Journal of Computer-Aided Molecular Design, 2001, 15, 129-144.	1.3	11
99	Biomimetic Synthesis of Lantibiotics. Chemistry - A European Journal, 2000, 6, 1455-1466.	1.7	79
100	Molecular dynamics of mouse and Syrian hamster PrP: Implications for activity. Proteins: Structure, Function and Bioinformatics, 2000, 38, 327-340.	1.5	32
101	Digitally filtered molecular dynamics: The frequency specific control of molecular dynamics simulations. Journal of Chemical Physics, 2000, 112, 2586-2597.	1.2	18
102	Biomimetic Synthesis of Lantibiotics. , 2000, 6, 1455.		2
103	Generation of OPLS-like charges from molecular electrostatic potential using restraints. Journal of Computational Chemistry, 1999, 20, 483-498.	1.5	25
104	Free energies of hydration using restrained electrostatic potential derived charges via free energy perturbations and linear response. Journal of Computational Chemistry, 1999, 20, 499-510.	1.5	19
105	Binding Constants of Neuraminidase Inhibitors:Â An Investigation of the Linear Interaction Energy Method. Journal of Medicinal Chemistry, 1999, 42, 5142-5152.	2.9	81
106	The Application of the Reaction-Field Method to the Calculation of Dielectric Constants. Molecular Simulation, 1998, 20, 159-178.	0.9	16
107	Monte Carlo Simulations for Proteins:Â Binding Affinities for Trypsinâ^'Benzamidine Complexes via Free-Energy Perturbations. Journal of Physical Chemistry B, 1997, 101, 9663-9669.	1.2	88
108	Stabilization of aCisAmide Bond in a Hostâ^'Guest Complex. Journal of the American Chemical Society, 1996, 118, 10220-10227.	6.6	69

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109	Generalized alteration of structure and parameters: A new method for free-energy perturbations in systems containing flexible degrees of freedom. Journal of Computational Chemistry, 1995, 16, 311-327.	1.5	30
110	An empirical boundary potential for water droplet simulations. Journal of Computational Chemistry, 1995, 16, 951-972.	1.5	72
111	Theoretical Calculation of a Solution Phase Torsional Free Energy Profile. Ï€-Ethylimidazole in Water. Molecular Simulation, 1993, 9, 369-383.	0.9	2
112	Atomic charges for variable molecular conformations. Journal of the American Chemical Society, 1992, 114, 9075-9079.	6.6	163
113	Theoretical determination of partition coefficients. Journal of the American Chemical Society, 1992, 114, 3634-3639.	6.6	65
114	Errors in free-energy perturbation calculations due to neglecting the conformational variation of atomic charges. Chemical Physics Letters, 1992, 199, 257-260.	1.2	35
115	Free Energy Calculations of Pharmaceutically Important Properties. Molecular Simulation, 1990, 5, 265-275.	0.9	8
116	Combinatorial Chemistry and the Grid. , 0, , 945-962.		10
117	On the Issues Impacting Reproducibility of Alchemical Free Energy Calculations. ACS Symposium Series, 0, , 109-125.	0.5	1