Jay W Ponder

List of Publications by Year
in descending order

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62 papers	12,246 citations	87723 38 h-index	123241 61 g-index
64 all docs	64 docs citations	64 times ranked	8782 citing authors

#	Article	IF	Citations
1	Computationally driven discovery of SARS-CoV-2 M^{pro}inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	3.7	21
2	AMOEBA binding free energies for the SAMPL7 TrimerTrip hostâ€“guest challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 79-93.	1.3	21
3	Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields Using GPUs and Multi-GPU Systems. Journal of Chemical Theory and Computation, 2021, 17, 2034-2053.	2.3	40
4	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. Journal of Chemical Theory and Computation, 2021, 17, 2323-2341.	2.3	10
5	Polarizable Water Potential Derived from a Model Electron Density. Journal of Chemical Theory and Computation, 2021, 17, 7056-7084.	2.3	26
6	Classical Pauli repulsion: An anisotropic, atomic multipole model. Journal of Chemical Physics, 2019, 150, 084104.	1.2	51
7	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 1, .	2.2	8
8	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. Journal of Chemical Theory and Computation, 2018, 14, 2084-2108.	2.3	178
9	Absolute binding free energies for the SAMPL6 cucurbit[8]uril hostâ€“guest challenge via the AMOEBA polarizable force field. Journal of Computer-Aided Molecular Design, 2018, 32, 1087-1095.	1.3	26
10	Tinker 8: Software Tools for Molecular Design. Journal of Chemical Theory and Computation, 2018, 14, 5273-5289.	2.3	403
11	A physically grounded damped dispersion model with particle mesh Ewald summation. Journal of Chemical Physics, 2018, 149, 084115.	1.2	18
12	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. Chemical Science, 2018, 9, 956-972.	3.7	190
13	Tinkerâ€OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. Journal of Computational Chemistry, 2017, 38, 2047-2055.	1.5	89
14	An optimized charge penetration model for use with the AMOEBA force field. Physical Chemistry Chemical Physics, 2017, 19, 276-291.	1.3	65
15	Truncated Conjugate Gradient: An Optimal Strategy for the Analytical Evaluation of the Many-Body Polarization Energy and Forces in Molecular Simulations. Journal of Chemical Theory and Computation, 2017, 13, 180-190.	2.3	34
16	An empirical extrapolation scheme for efficient treatment of induced dipoles. Journal of Chemical Physics, 2016, 145, 164101.	1.2	27
17	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. Journal of Chemical Physics, 2016, 145, 124106.	1.2	46
18	Calculating binding free energies of hostâ€“guest systems using the AMOEBA polarizable force field. Physical Chemistry Chemical Physics, 2016, 18, 30261-30269.	1.3	44

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19	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	1.2	77
20	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general shortâ€range penetration correction up to quadrupoles. Journal of Computational Chemistry, 2016, 37, 494-506.	1.5	26
21	High-Resolution Crystal Structures of Protein Helices Reconciled with Three-Centered Hydrogen Bonds and Multipole Electrostatics. PLoS ONE, 2015, 10, e0123146.	1.1	25
22	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. Journal of Chemical Theory and Computation, 2015, 11, 2609-2618.	2.3	93
23	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. Journal of Physical Chemistry B, 2015, 119, 9423-9437.	1.2	183
24	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. Journal of Chemical Theory and Computation, 2015, 11, 5326-5339.	2.3	26
25	An Angular Overlap Model for Cu(II) Ion in the AMOEBA Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 298-311.	2.3	28
26	Helix stability of oligoglycine, oligoalanine, and oligo-Î²-alanine dodecamers reflected by hydrogen-bond persistence. Proteins: Structure, Function and Bioinformatics, 2014, 82, 3043-3061.	1.5	15
27	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	2.3	524
28	Systematic Improvement of a Classical Molecular Model of Water. Journal of Physical Chemistry B, 2013, 117, 9956-9972.	1.2	279
29	A valence bond model for aqueous Cu(II) and Zn(II) ions in the AMOEBA polarizable force field. Journal of Computational Chemistry, 2013, 34, 739-749.	1.5	34
30	Molecular Dynamics of Î²-Hairpin Models of Epigenetic Recognition Motifs. Journal of the American Chemical Society, 2012, 134, 15970-15978.	6.6	29
31	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. Journal of Chemical Theory and Computation, 2011, 7, 3143-3161.	2.3	385
32	MSCALE: A General Utility for Multiscale Modeling. Journal of Chemical Theory and Computation, 2011, 7, 1208-1219.	2.3	41
33	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	1.5	69
34	Current Status of the AMOEBA Polarizable Force Field. Journal of Physical Chemistry B, 2010, 114, 2549-2564.	1.2	1,093
35	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. Journal of Chemical Physics, 2007, 126, 124114.	1.2	79
36	Polarizable Atomic Multipole Solutes in a Generalized Kirkwood Continuum. Journal of Chemical Theory and Computation, 2007, 3, 2083-2097.	2.3	66

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37	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. International Journal of Quantum Chemistry, 2007, 107, 1390-1395.	1.0	81
38	Temperature and Pressure Dependence of the AMOEBA Water Model. Journal of Physical Chemistry B, 2004, 108, 13427-13437.	1.2	191
39	Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field. Journal of the American Chemical Society, 2003, 125, 15671-15682.	6.6	474
40	Force Fields for Protein Simulations. Advances in Protein Chemistry, 2003, 66, 27-85.	4.4	1,560
41	Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation. Journal of Physical Chemistry B, 2003, 107, 5933-5947.	1.2	1,270
42	Consistent treatment of inter- and intramolecular polarization in molecular mechanics calculations. Journal of Computational Chemistry, 2002, 23, 1497-1506.	1.5	545
43	Exploring the similarities between potential smoothing and simulated annealing. Journal of Computational Chemistry, 2000, 21, 531-552.	1.5	30
44	Binding of retinol induces changes in rat cellular retinol-binding protein II conformation and backbone dynamics. Journal of Molecular Biology, 2000, 300, 619-632.	2.0	44
45	A potential smoothing algorithm accurately predicts transmembrane helix packing. Nature Structural Biology, 1999, 6, 50-55.	9.7	57
46	The structure and dynamics of rat apo-cellular retinol-binding protein II in solution: comparison with the X-ray structure 1 1Edited by P. E. Wright. Journal of Molecular Biology, 1999, 286, 1179-1195.	2.0	46
47	Ab Initio fold prediction of small helical proteins using distance geometry and knowledge-based scoring functions 1 1Edited by F. Cohen. Journal of Molecular Biology, 1999, 290, 267-281.	2.0	89
48	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions. Journal of Computational Chemistry, 1998, 19, 548-573.	1.5	83
49	Accuracy of side-chain prediction upon near-native protein backbones generated by ab initio folding methods. , 1998, 33, 204-217.		42
50	Distance geometry generates nativeâ€like folds for small helical proteins using the consensus distances of predicted protein structures. Protein Science, 1998, 7, 1998-2003.	3.1	26
51	Analysis and Application of Potential Energy Smoothing and Search Methods for Global Optimization. Journal of Physical Chemistry B, 1998, 102, 9725-9742.	1.2	239
52	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions. Journal of Computational Chemistry, 1998, 19, 548.	1.5	4
53	Calculation of the reaction field due to off-center point multipoles. Journal of Chemical Physics, 1997, 107, 481-492.	1.2	55
54	The NMR Solution Structure of Intestinal Fatty Acid-binding Protein Complexed with Palmitate: Application of a Novel Distance Geometry Algorithm. Journal of Molecular Biology, 1996, 264, 585-602.	2.0	159

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55	Accurate modeling of the intramolecular electrostatic energy of proteins. Journal of Computational Chemistry, 1995, 16, 791-816.	1.5	228
56	Crystallization and Initial X-ray Crystallographic Characterization of Recombinant Bovine Inositol Polyphosphate 1-Phosphatase Produced in Spodoptera frugiperda Cells. Journal of Molecular Biology, 1994, 236, 584-589.	2.0	16
57	Algorithms for calculating excluded volume and its derivatives as a function of molecular conformation and their use in energy minimization. Journal of Computational Chemistry, 1991, 12, 402-409.	1.5	183
58	Tertiary templates for proteins. Journal of Molecular Biology, 1987, 193, 775-791.	2.0	1,496
59	An efficient newton-like method for molecular mechanics energy minimization of large molecules. Journal of Computational Chemistry, 1987, 8, 1016-1024.	1.5	854
60	The stereochemistry and biosynthesis of hybridalactone, an eicosanoid from. Tetrahedron Letters, 1984, 25, 1015-1018.	0.7	36
61	Stereochemistry of the hygrolidins. Tetrahedron Letters, 1984, 25, 4325-4328.	0.7	59
62	Metal-ammonia reduction of triptycene and related benzobarrelene derivatives. Journal of Organic Chemistry, 1979, 44, 4594-4597.	1.7	10