

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	Force Fields for Protein Simulations. <i>Advances in Protein Chemistry</i> , 2003, 66, 27-85.	4.4	1,560
2	Tertiary templates for proteins. <i>Journal of Molecular Biology</i> , 1987, 193, 775-791.	2.0	1,496
3	Polarizable Atomic Multipole Water Model for Molecular Mechanics Simulation. <i>Journal of Physical Chemistry B</i> , 2003, 107, 5933-5947.	1.2	1,270
4	Current Status of the AMOEBA Polarizable Force Field. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2549-2564.	1.2	1,093
5	An efficient newton-like method for molecular mechanics energy minimization of large molecules. <i>Journal of Computational Chemistry</i> , 1987, 8, 1016-1024.	1.5	854
6	Consistent treatment of inter- and intramolecular polarization in molecular mechanics calculations. <i>Journal of Computational Chemistry</i> , 2002, 23, 1497-1506.	1.5	545
7	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4046-4063.	2.3	524
8	Ion Solvation Thermodynamics from Simulation with a Polarizable Force Field. <i>Journal of the American Chemical Society</i> , 2003, 125, 15671-15682.	6.6	474
9	Tinker 8: Software Tools for Molecular Design. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5273-5289.	2.3	403
10	Polarizable Atomic Multipole-Based Molecular Mechanics for Organic Molecules. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3143-3161.	2.3	385
11	Systematic Improvement of a Classical Molecular Model of Water. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9956-9972.	1.2	279
12	Analysis and Application of Potential Energy Smoothing and Search Methods for Global Optimization. <i>Journal of Physical Chemistry B</i> , 1998, 102, 9725-9742.	1.2	239
13	Accurate modeling of the intramolecular electrostatic energy of proteins. <i>Journal of Computational Chemistry</i> , 1995, 16, 791-816.	1.5	228
14	Temperature and Pressure Dependence of the AMOEBA Water Model. <i>Journal of Physical Chemistry B</i> , 2004, 108, 13427-13437.	1.2	191
15	Tinker-HP: a massively parallel molecular dynamics package for multiscale simulations of large complex systems with advanced point dipole polarizable force fields. <i>Chemical Science</i> , 2018, 9, 956-972.	3.7	190
16	Algorithms for calculating excluded volume and its derivatives as a function of molecular conformation and their use in energy minimization. <i>Journal of Computational Chemistry</i> , 1991, 12, 402-409.	1.5	183
17	Revised Parameters for the AMOEBA Polarizable Atomic Multipole Water Model. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9423-9437.	1.2	183
18	AMOEBA Polarizable Atomic Multipole Force Field for Nucleic Acids. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2084-2108.	2.3	178

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19	The NMR Solution Structure of Intestinal Fatty Acid-binding Protein Complexed with Palmitate: Application of a Novel Distance Geometry Algorithm. <i>Journal of Molecular Biology</i> , 1996, 264, 585-602.	2.0	159
20	General Model for Treating Short-Range Electrostatic Penetration in a Molecular Mechanics Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2609-2618.	2.3	93
21	Ab Initio fold prediction of small helical proteins using distance geometry and knowledge-based scoring functions 1 Edited by F. Cohen. <i>Journal of Molecular Biology</i> , 1999, 290, 267-281.	2.0	89
22	Tinkerâ€OpenMM: Absolute and relative alchemical free energies using AMOEBA on GPUs. <i>Journal of Computational Chemistry</i> , 2017, 38, 2047-2055.	1.5	89
23	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions. <i>Journal of Computational Chemistry</i> , 1998, 19, 548-573.	1.5	83
24	Force field modeling of conformational energies: Importance of multipole moments and intramolecular polarization. <i>International Journal of Quantum Chemistry</i> , 2007, 107, 1390-1395.	1.0	81
25	Polarizable atomic multipole solutes in a Poisson-Boltzmann continuum. <i>Journal of Chemical Physics</i> , 2007, 126, 124114.	1.2	79
26	Advanced Potential Energy Surfaces for Molecular Simulation. <i>Journal of Physical Chemistry B</i> , 2016, 120, 9811-9832.	1.2	77
27	Multipole electrostatics in hydration free energy calculations. <i>Journal of Computational Chemistry</i> , 2011, 32, 967-977.	1.5	69
28	Polarizable Atomic Multipole Solute in a Generalized Kirkwood Continuum. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2083-2097.	2.3	66
29	An optimized charge penetration model for use with the AMOEBA force field. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 276-291.	1.3	65
30	Stereochemistry of the hygrolydins. <i>Tetrahedron Letters</i> , 1984, 25, 4325-4328.	0.7	59
31	A potential smoothing algorithm accurately predicts transmembrane helix packing. <i>Nature Structural Biology</i> , 1999, 6, 50-55.	9.7	57
32	Calculation of the reaction field due to off-center point multipoles. <i>Journal of Chemical Physics</i> , 1997, 107, 481-492.	1.2	55
33	Classical Pauli repulsion: An anisotropic, atomic multipole model. <i>Journal of Chemical Physics</i> , 2019, 150, 084104.	1.2	51
34	The structure and dynamics of rat apo-cellular retinol-binding protein II in solution: comparison with the X-ray structure 1 Edited by P. E. Wright. <i>Journal of Molecular Biology</i> , 1999, 286, 1179-1195.	2.0	46
35	TINKTEP: A fully self-consistent, mutually polarizable QM/MM approach based on the AMOEBA force field. <i>Journal of Chemical Physics</i> , 2016, 145, 124106.	1.2	46
36	Binding of retinol induces changes in rat cellular retinol-binding protein II conformation and backbone dynamics. <i>Journal of Molecular Biology</i> , 2000, 300, 619-632.	2.0	44

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37	Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 30261-30269.	1.3	44
38	Accuracy of side-chain prediction upon near-native protein backbones generated by ab initio folding methods. , 1998, 33, 204-217.		42
39	MSCALE: A General Utility for Multiscale Modeling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1208-1219.	2.3	41
40	Tinker-HP: Accelerating Molecular Dynamics Simulations of Large Complex Systems with Advanced Point Dipole Polarizable Force Fields Using GPUs and Multi-GPU Systems. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2034-2053.	2.3	40
41	The stereochemistry and biosynthesis of hybridalactone, an eicosanoid from. <i>Tetrahedron Letters</i> , 1984, 25, 1015-1018.	0.7	36
42	A valence bond model for aqueous Cu(II) and Zn(II) ions in the AMOEBA polarizable force field. <i>Journal of Computational Chemistry</i> , 2013, 34, 739-749.	1.5	34
43	Truncated Conjugate Gradient: An Optimal Strategy for the Analytical Evaluation of the Many-Body Polarization Energy and Forces in Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 180-190.	2.3	34
44	Exploring the similarities between potential smoothing and simulated annealing. <i>Journal of Computational Chemistry</i> , 2000, 21, 531-552.	1.5	30
45	Molecular Dynamics of β -Hairpin Models of Epigenetic Recognition Motifs. <i>Journal of the American Chemical Society</i> , 2012, 134, 15970-15978.	6.6	29
46	An Angular Overlap Model for Cu(II) Ion in the AMOEBA Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 298-311.	2.3	28
47	An empirical extrapolation scheme for efficient treatment of induced dipoles. <i>Journal of Chemical Physics</i> , 2016, 145, 164101.	1.2	27
48	Distance geometry generates native-like folds for small helical proteins using the consensus distances of predicted protein structures. <i>Protein Science</i> , 1998, 7, 1998-2003.	3.1	26
49	Polarizable Multipole-Based Force Field for Dimethyl and Trimethyl Phosphate. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5326-5339.	2.3	26
50	Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles. <i>Journal of Computational Chemistry</i> , 2016, 37, 494-506.	1.5	26
51	Absolute binding free energies for the SAMPL6 cucurbit[8]uril host-guest challenge via the AMOEBA polarizable force field. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1087-1095.	1.3	26
52	Polarizable Water Potential Derived from a Model Electron Density. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7056-7084.	2.3	26
53	High-Resolution Crystal Structures of Protein Helices Reconciled with Three-Centered Hydrogen Bonds and Multipole Electrostatics. <i>PLoS ONE</i> , 2015, 10, e0123146.	1.1	25
54	AMOEBA binding free energies for the SAMPL7 TrimerTrip host-guest challenge. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 79-93.	1.3	21

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55	Computationally driven discovery of SARS-CoV-2 M ^{pro} inhibitors: from design to experimental validation. <i>Chemical Science</i> , 2022, 13, 3674-3687.	3.7	21
56	A physically grounded damped dispersion model with particle mesh Ewald summation. <i>Journal of Chemical Physics</i> , 2018, 149, 084115.	1.2	18
57	Crystallization and Initial X-ray Crystallographic Characterization of Recombinant Bovine Inositol Polyphosphate 1-Phosphatase Produced in <i>Spodoptera frugiperda</i> Cells. <i>Journal of Molecular Biology</i> , 1994, 236, 584-589.	2.0	16
58	Helix stability of oligoglycine, oligoalanine, and oligo- β -alanine dodecamers reflected by hydrogen-bond persistence. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 3043-3061.	1.5	15
59	Metal-ammonia reduction of triptycene and related benzobarrelene derivatives. <i>Journal of Organic Chemistry</i> , 1979, 44, 4594-4597.	1.7	10
60	Implicit Solvents for the Polarizable Atomic Multipole AMOEBA Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2323-2341.	2.3	10
61	Raising the Performance of the Tinker-HP Molecular Modeling Package [Article v1.0]. <i>Living Journal of Computational Molecular Science</i> , 2019, 1, .	2.2	8
62	Protein structure prediction using a combination of sequence homology and global energy minimization: II. Energy functions. <i>Journal of Computational Chemistry</i> , 1998, 19, 548.	1.5	4