

David A Pearlman

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60
papers

5,945
citations

33
h-index

61
g-index

61
ext. papers

6,492
ext. citations

5.5
avg, IF

5.42
L-index

#	Paper	IF	Citations
60	AMBER, a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules. <i>Computer Physics Communications</i> , 1995 , 91, 1-41	4.2	2509
59	Benzene Dimer: A Good Model for π -Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. <i>Journal of the American Chemical Society</i> , 1996 , 118, 11217-11224	16.4	265
58	Are free energy calculations useful in practice? A comparison with rapid scoring functions for the p38 MAP kinase protein system. <i>Journal of Medicinal Chemistry</i> , 2001 , 44, 3417-23	8.3	196
57	Molecular models for DNA damaged by photoreaction. <i>Science</i> , 1985 , 227, 1304-8	33.3	184
56	Evaluating the molecular mechanics poisson-boltzmann surface area free energy method using a congeneric series of ligands to p38 MAP kinase. <i>Journal of Medicinal Chemistry</i> , 2005 , 48, 7796-807	8.3	164
55	A Comparison of Alternative Approaches to Free Energy Calculations. <i>The Journal of Physical Chemistry</i> , 1994 , 98, 1487-1493		163
54	Are time-averaged restraints necessary for nuclear magnetic resonance refinement? A model study for DNA. <i>Journal of Molecular Biology</i> , 1991 , 220, 457-79	6.5	133
53	The overlooked bond-stretching contribution in free energy perturbation calculations. <i>Journal of Chemical Physics</i> , 1991 , 94, 4532-4545	3.9	132
52	Applying physics-based scoring to calculate free energies of binding for single amino acid mutations in protein-protein complexes. <i>PLoS ONE</i> , 2013 , 8, e82849	3.7	116
51	Ionic charging free energies: Spherical versus periodic boundary conditions. <i>Journal of Chemical Physics</i> , 1998 , 109, 10921-10935	3.9	114
50	Antibody structure determination using a combination of homology modeling, energy-based refinement, and loop prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 1646-55	4.2	110
49	The lag between the Hamiltonian and the system configuration in free energy perturbation calculations. <i>Journal of Chemical Physics</i> , 1989 , 91, 7831-7839	3.9	110
48	Simulation of the solvation free energies for methane, ethane, and propane and corresponding amino acid dipeptides: a critical test of the bond-PMF correction, a new set of hydrocarbon parameters, and the gas phase-water hydrophobicity scale. <i>Journal of the American Chemical Society</i> , 1992 , 114, 6798-6801	16.4	107
47	A new method for carrying out free energy perturbation calculations: Dynamically modified windows. <i>Journal of Chemical Physics</i> , 1989 , 90, 2460-2470	3.9	106
46	CONCERTS: dynamic connection of fragments as an approach to de novo ligand design. <i>Journal of Medicinal Chemistry</i> , 1996 , 39, 1651-63	8.3	98
45	Improved scoring of ligand-protein interactions using OWFEG free energy grids. <i>Journal of Medicinal Chemistry</i> , 2001 , 44, 502-11	8.3	88
44	Molecular Dynamics Potential of Mean Force Calculations: A Study of the Toluene π -Ammonium π -Cation Interactions. <i>Journal of the American Chemical Society</i> , 1996 , 118, 2998-3005	16.4	85

43	Free Energy Calculations. The Long and Winding Gilded Road. <i>Molecular Simulation</i> , 2002 , 28, 1-12	2	79
42	CONCEPTS: New dynamic algorithm for de novo drug suggestion. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1184-1193	3.5	67
41	Determining the contributions of constraints in free energy calculations: Development, characterization, and recommendations. <i>Journal of Chemical Physics</i> , 1993 , 98, 8946-8957	3.9	65
40	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 5595-5623	6.1	56
39	Predicting the Effect of Amino Acid Single-Point Mutations on Protein Stability-Large-Scale Validation of MD-Based Relative Free Energy Calculations. <i>Journal of Molecular Biology</i> , 2017 , 429, 948-963	6.5	54
38	Rigorous Free Energy Simulations in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 4153-4169	6.1	54
37	Alternative approaches to potential of mean force calculations: Free energy perturbation versus thermodynamic integration. Case study of some representative nonpolar interactions. <i>Journal of Computational Chemistry</i> , 1996 , 17, 1112-1131	3.5	52
36	Free energy derivatives: A new method for probing the convergence problem in free energy calculations. <i>Journal of Computational Chemistry</i> , 1994 , 15, 105-123	3.5	51
35	Atomic charges for DNA constituents derived from single-crystal X-ray diffraction data. <i>Journal of Molecular Biology</i> , 1990 , 211, 171-87	6.5	50
34	How is an NMR structure best defined? An analysis of molecular dynamics distance-based approaches. <i>Journal of Biomolecular NMR</i> , 1994 , 4, 1-16	3	49
33	Conformational studies of nucleic acids. II. The conformational energetics of commonly occurring nucleosides. <i>Journal of Biomolecular Structure and Dynamics</i> , 1985 , 3, 99-125	3.6	42
32	Determinations of atomic partial charges for nucleic acid constituents from x-ray diffraction data. I. 2-Deoxythymidine-5-phosphate. <i>Biopolymers</i> , 1985 , 24, 327-57	2.2	41
31	Determination of the differential effects of hydrogen bonding and water release on the binding of FK506 to native and Tyr82-->Phe82 FKBP-12 proteins using free energy simulations. <i>Journal of Molecular Biology</i> , 1995 , 248, 696-717	6.5	40
30	Structure-based approach to the prediction of disulfide bonds in proteins. <i>Protein Engineering, Design and Selection</i> , 2014 , 27, 365-74	1.9	39
29	The calculated free energy effects of 5-methyl cytosine on the B to Z transition in DNA. <i>Biopolymers</i> , 1990 , 29, 1193-209	2.2	33
28	Solution structure of [d(GTATATAC)] ₂ via restrained molecular dynamics simulations with nuclear magnetic resonance constraints derived from relaxation matrix analysis of two-dimensional nuclear Overhauser effect experiments. <i>Journal of Molecular Biology</i> , 1991 , 221, 271-92	6.5	33
27	Free energy grids: a practical qualitative application of free energy perturbation to ligand design using the OWFEG method. <i>Journal of Medicinal Chemistry</i> , 1999 , 42, 4313-24	8.3	32
26	Physics-based enzyme design: predicting binding affinity and catalytic activity. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014 , 82, 3397-409	4.2	29

25	How well do time-averaged J-coupling restraints work?. <i>Journal of Biomolecular NMR</i> , 1994 , 4, 279-99	3	29
24	Free energy perturbation calculations involving potential function changes. <i>Journal of Computational Chemistry</i> , 1992 , 13, 362-370	3.5	29
23	Protein solution structure calculations in solution: solvated molecular dynamics refinement of calbindin D9k. <i>Journal of Biomolecular NMR</i> , 1997 , 10, 231-43	3	28
22	FINGAR: A new genetic algorithm-based method for fitting NMR data. <i>Journal of Biomolecular NMR</i> , 1996 , 8, 49-66	3	27
21	AAK1 identified as an inhibitor of neuregulin-1/ErbB4-dependent neurotrophic factor signaling using integrative chemical genomics and proteomics. <i>Chemistry and Biology</i> , 2011 , 18, 891-906		26
20	Conformation of FK506 in X-ray structures of its complexes with human recombinant FKBP12 mutants. <i>Bioorganic and Medicinal Chemistry Letters</i> , 1995 , 5, 1983-1988	2.9	26
19	Evaluating the assumptions underlying force field development and application using free energy conformational maps for nucleosides. <i>Journal of the American Chemical Society</i> , 1991 , 113, 7167-7177	16.4	26
18	Calculations of the relative free energies of aqueous solvation of several fluorocarbons: A test of the bond potential of mean force correction. <i>Journal of Chemical Physics</i> , 1993 , 99, 9103-9110	3.9	25
17	Conformational studies of nucleic acids. I. A rapid and direct method for generating furanose coordinates from the pseudorotation angle. <i>Journal of Biomolecular Structure and Dynamics</i> , 1985 , 3, 85-98	3.6	25
16	Comparison of solution structures of mutant bovine pancreatic trypsin inhibitor proteins using two-dimensional nuclear magnetic resonance. <i>Protein Science</i> , 1992 , 1, 91-106	6.3	21
15	Conformational studies of nucleic acids: III. Empirical multiple correlation functions for nucleic acid torsion angles. <i>Journal of Biomolecular Structure and Dynamics</i> , 1986 , 4, 49-67	3.6	19
14	Effects of nucleotide bromination on the stabilities of Z-RNA and Z-DNA: a molecular mechanics/thermodynamic perturbation study. <i>Biopolymers</i> , 1989 , 28, 1939-57	2.2	17
13	Conformational studies of nucleic acids: IV. The conformational energetics of oligonucleotides: d(ApApApA) and ApApApA. <i>Journal of Biomolecular Structure and Dynamics</i> , 1986 , 4, 69-98	3.6	17
12	Walking on the free energy hypersurface of the 18-crown-6 ion system using free energy derivatives. <i>Journal of Chemical Physics</i> , 1994 , 101, 627-633	3.9	16
11	Automated detection of problem restraints in NMR data sets using the FINGAR genetic algorithm method. <i>Journal of Biomolecular NMR</i> , 1999 , 13, 325-35	3	12
10	Free energy perturbation calculations on parallel computers: Demonstrations of scalable linear speedup. <i>Journal of Computational Chemistry</i> , 1994 , 15, 351-373	3.5	12
9	Solution structure of FK506 bound to the R42K, H87V double mutant of FKBP-12. <i>Biochemistry</i> , 1994 , 33, 13571-80	3.2	12
8	Conformational studies of nucleic acids. V. Sequence specificities in the conformational energetics of oligonucleotides: the homo-tetramers. <i>Biopolymers</i> , 1988 , 27, 59-77	2.2	7

7	FURSMASA: a new approach to rapid scoring functions that uses a MD-averaged potential energy grid and a solvent-accessible surface area term with parameters GA fit to experimental data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 71, 1519-38	4.2	6
6	Predicting mutations deleterious to function in beta-lactamase TEM1 using MM-GBSA. <i>PLoS ONE</i> , 2019 , 14, e0214015	3.7	4
5	Free energy component analysis: application to the "Z-phobicity" of A-T base pairs. <i>Journal of Biomolecular Structure and Dynamics</i> , 1993 , 11, 303-11	3.6	4
4	Quantum simulations of SARS-CoV-2 main protease M enable high-quality scoring of diverse ligands. <i>Journal of Computer-Aided Molecular Design</i> , 2021 , 35, 963-971	4.2	4
3	Practical applications of time-averaged restrained molecular dynamics to ligand-receptor systems: FK506 bound to the Q50R,A95H,K98I triple mutant of FKBP-13. <i>Journal of Biomolecular NMR</i> , 1996 , 8, 67-76	3	3
2	Structure of DNA damaged by UV and psoralen. <i>Biochemical Pharmacology</i> , 1988 , 37, 1791	6	2
1	AMBER: A Program for Simulation of Biological and Organic Molecules		2