David A Pearlman

List of Publications by Year in Descending Order

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	Quantum simulations of SARS-CoV-2 main protease M enable high-quality scoring of diverse ligands. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 963-971	4.2	4
59	Rigorous Free Energy Simulations in Virtual Screening. *Journal of Chemical Information and Modeling*, **2020**, 60, 4153-4169	6.1	54
58	Alchemical Binding Free Energy Calculations in AMBER20: Advances and Best Practices for Drug Discovery. *Journal of Chemical Information and Modeling*, **2020**, 60, 5595-5623	6.1	56
57	Predicting mutations deleterious to function in beta-lactamase TEM1 using MM-GBSA. *PLoS ONE*, **2019**, 14, e0214015	3.7	4
56	Predicting the Effect of Amino Acid Single-Point Mutations on Protein Stability-Large-Scale Validation of MD-Based Relative Free Energy Calculations. *Journal of Molecular Biology*, **2017**, 429, 948-963	6.5	54
55	Antibody structure determination using a combination of homology modeling, energy-based refinement, and loop prediction. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 1646-55	4.2	110
54	Physics-based enzyme design: predicting binding affinity and catalytic activity. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 3397-409	4.2	29
53	Structure-based approach to the prediction of disulfide bonds in proteins. *Protein Engineering, Design and Selection*, **2014**, 27, 365-74	1.9	39
52	Applying physics-based scoring to calculate free energies of binding for single amino acid mutations in protein-protein complexes. *PLoS ONE*, **2013**, 8, e82849	3.7	116
51	AAK1 identified as an inhibitor of neuregulin-1/ErbB4-dependent neurotrophic factor signaling using integrative chemical genomics and proteomics. *Chemistry and Biology*, **2011**, 18, 891-906		26
50	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. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1519-38	4.2	6
49	Evaluating the molecular mechanics poisson-boltzmann surface area free energy method using a congeneric series of ligands to p38 MAP kinase. *Journal of Medicinal Chemistry*, **2005**, 48, 7796-807	8.3	164
48	Free Energy Calculations. The Long and Winding Gilded Road. *Molecular Simulation*, **2002**, 28, 1-12	2	79
47	Are free energy calculations useful in practice? A comparison with rapid scoring functions for the p38 MAP kinase protein system. *Journal of Medicinal Chemistry*, **2001**, 44, 3417-23	8.3	196
46	Improved scoring of ligand-protein interactions using OWFEG free energy grids. *Journal of Medicinal Chemistry*, **2001**, 44, 502-11	8.3	88
45	Automated detection of problem restraints in NMR data sets using the FINGAR genetic algorithm method. *Journal of Biomolecular NMR*, **1999**, 13, 325-35	3	12
44	Free energy grids: a practical qualitative application of free energy perturbation to ligand design using the OWFEG method. *Journal of Medicinal Chemistry*, **1999**, 42, 4313-24	8.3	32

43	Ionic charging free energies: Spherical versus periodic boundary conditions. *Journal of Chemical Physics*, **1998**, 109, 10921-10935	3.9	114
42	Protein solution structure calculations in solution: solvated molecular dynamics refinement of calbindin D9k. *Journal of Biomolecular NMR*, **1997**, 10, 231-43	3	28
41	Molecular Dynamics Potential of Mean Force Calculations: A Study of the Toluene□Ammonium □Cation Interactions. *Journal of the American Chemical Society*, **1996**, 118, 2998-3005	16.4	85
40	Benzene Dimer: A Good Model for □Interactions in Proteins? A Comparison between the Benzene and the Toluene Dimers in the Gas Phase and in an Aqueous Solution. *Journal of the American Chemical Society*, **1996**, 118, 11217-11224	16.4	265
39	CONCERTS: dynamic connection of fragments as an approach to de novo ligand design. *Journal of Medicinal Chemistry*, **1996**, 39, 1651-63	8.3	98
38	Alternative approaches to potential of mean force calculations: Free energy perturbation versus thermodynamic integration. Case study of some representative nonpolar interactions. *Journal of Computational Chemistry*, **1996**, 17, 1112-1131	3.5	52
37	FINGAR: A new genetic algorithm-based method for fitting NMR data. *Journal of Biomolecular NMR*, **1996**, 8, 49-66	3	27
36	Practical applications of time-averaged restrained molecular dynamics to ligand-receptor systems: FK506 bound to the Q50R,A95H,K98I triple mutant of FKBP-13. *Journal of Biomolecular NMR*, **1996**, 8, 67-76	3	3
35	Conformation of FK506 in X-ray structures of its complexes with human recombinant FKBP12 mutants. *Bioorganic and Medicinal Chemistry Letters*, **1995**, 5, 1983-1988	2.9	26
34	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. *Journal of Molecular Biology*, **1995**, 248, 696-717	6.5	40
33	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. *Computer Physics Communications*, **1995**, 91, 1-41	4.2	2509
32	Walking on the free energy hypersurface of the 18-crown-6 ion system using free energy derivatives. *Journal of Chemical Physics*, **1994**, 101, 627-633	3.9	16
31	How well do time-averaged J-coupling restraints work?. *Journal of Biomolecular NMR*, **1994**, 4, 279-99	3	29
30	How is an NMR structure best defined? An analysis of molecular dynamics distance-based approaches. *Journal of Biomolecular NMR*, **1994**, 4, 1-16	3	49
29	Free energy derivatives: A new method for probing the convergence problem in free energy calculations. *Journal of Computational Chemistry*, **1994**, 15, 105-123	3.5	51
28	Free energy perturbation calculations on parallel computers: Demonstrations of scalable linear speedup. *Journal of Computational Chemistry*, **1994**, 15, 351-373	3.5	12
27	A Comparison of Alternative Approaches to Free Energy Calculations. *The Journal of Physical Chemistry*, **1994**, 98, 1487-1493		163
26	Solution structure of FK506 bound to the R42K, H87V double mutant of FKBP-12. *Biochemistry*, **1994**, 33, 13571-80	3.2	12

25	Calculations of the relative free energies of aqueous solvation of several fluorocarbons: A test of the bond potential of mean force correction. *Journal of Chemical Physics*, **1993**, 99, 9103-9110	3.9	25
24	Determining the contributions of constraints in free energy calculations: Development, characterization, and recommendations. *Journal of Chemical Physics*, **1993**, 98, 8946-8957	3.9	65
23	Free energy component analysis: application to the "Z-phobicity" of A-T base pairs. *Journal of Biomolecular Structure and Dynamics*, **1993**, 11, 303-11	3.6	4
22	CONCEPTS: New dynamic algorithm for de novo drug suggestion. *Journal of Computational Chemistry*, **1993**, 14, 1184-1193	3.5	67
21	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. *Journal of the American Chemical Society*, **1992**, 114, 6798-6801	16.4	107
20	Comparison of solution structures of mutant bovine pancreatic trypsin inhibitor proteins using two-dimensional nuclear magnetic resonance. *Protein Science*, **1992**, 1, 91-106	6.3	21
19	Free energy perturbation calculations involving potential function changes. *Journal of Computational Chemistry*, **1992**, 13, 362-370	3.5	29
18	The overlooked bond-stretching contribution in free energy perturbation calculations. *Journal of Chemical Physics*, **1991**, 94, 4532-4545	3.9	132
17	Evaluating the assumptions underlying force field development and application using free energy conformational maps for nucleosides. *Journal of the American Chemical Society*, **1991**, 113, 7167-7177	16.4	26
16	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. *Journal of Molecular Biology*, **1991**, 221, 271-92	6.5	33
15	Are time-averaged restraints necessary for nuclear magnetic resonance refinement? A model study for DNA. *Journal of Molecular Biology*, **1991**, 220, 457-79	6.5	133
14	The calculated free energy effects of 5-methyl cytosine on the B to Z transition in DNA. *Biopolymers* , **1990**, 29, 1193-209	2.2	33
13	Atomic charges for DNA constituents derived from single-crystal X-ray diffraction data. *Journal of Molecular Biology*, **1990**, 211, 171-87	6.5	50
12	A new method for carrying out free energy perturbation calculations: Dynamically modified windows. *Journal of Chemical Physics*, **1989**, 90, 2460-2470	3.9	106
11	The lag between the Hamiltonian and the system configuration in free energy perturbation calculations. *Journal of Chemical Physics*, **1989**, 91, 7831-7839	3.9	110
10	Effects of nucleotide bromination on the stabilities of Z-RNA and Z-DNA: a molecular mechanics/thermodynamic perturbation study. *Biopolymers*, **1989**, 28, 1939-57	2.2	17
9	Conformational studies of nucleic acids. V. Sequence specificities in the conformational energetics of oligonucleotides: the homo-tetramers. *Biopolymers*, **1988**, 27, 59-77	2.2	7
8	Structure of DNA damaged by UV and psoralen. *Biochemical Pharmacology*, **1988**, 37, 1791	6	2

7	Conformational studies of nucleic acids: IV. The conformational energetics of oligonucleotides: d(ApApApA) and ApApApA. *Journal of Biomolecular Structure and Dynamics*, **1986**, 4, 69-98	3.6	17
6	Conformational studies of nucleic acids: III. Empirical multiple correlation functions for nucleic acid torsion angles. *Journal of Biomolecular Structure and Dynamics*, **1986**, 4, 49-67	3.6	19
5	Determinations of atomic partial charges for nucleic acid constituents from x-ray diffraction data. I. 2Q-Deoxycytidine-5Q-monophosphate. *Biopolymers*, **1985**, 24, 327-57	2.2	41
4	Conformational studies of nucleic acids. II. The conformational energetics of commonly occurring nucleosides. *Journal of Biomolecular Structure and Dynamics*, **1985**, 3, 99-125	3.6	42
3	Molecular models for DNA damaged by photoreaction. *Science*, **1985**, 227, 1304-8	33.3	184
2	Conformational studies of nucleic acids. I. A rapid and direct method for generating furanose coordinates from the pseudorotation angle. *Journal of Biomolecular Structure and Dynamics*, **1985**, 3, 85-98	3.6	25
1	AMBER: A Program for Simulation of Biological and Organic Molecules		2