David A Case

List of Publications by Year in Descending Order

254 papers	63,737 citations	87 h-index	252 g-index
272 ext. papers	71,512 ext. citations	7.8 avg, IF	7.68 L-index

#	Paper	IF	Citations
254	Integral equation models for solvent in macromolecular crystals.. *Journal of Chemical Physics*, **2022**, 156, 014801	3.9	1
253	Simulations of Kindlin-2 PIP binding domains reveal protonation-dependent membrane binding modes. *Biophysical Journal*, **2021**,	2.9	1
252	Refinement of RNA Structures Using Amber Force Fields. *Crystals*, **2021**, 11,	2.3	1
251	Molecular dynamics analysis of a flexible loop at the binding interface of the SARS-CoV-2 spike protein receptor-binding domain. *Proteins: Structure, Function and Bioinformatics*, **2021**,	4.2	9
250	A quantitative model predicts how mA reshapes the kinetic landscape of nucleic acid hybridization and conformational transitions. *Nature Communications*, **2021**, 12, 5201	17.4	8
249	Deleterious effects of carbon-carbon dipolar coupling on RNA NMR dynamics. *Journal of Biomolecular NMR*, **2020**, 74, 321-331	3	7
248	Diffuse X-ray scattering from correlated motions in a protein crystal. *Nature Communications*, **2020**, 11, 1271	17.4	12
247	The Interplay between Molten Globules and Heme Disassociation Defines Human Hemoglobin Disassembly. *Biophysical Journal*, **2020**, 118, 1381-1400	2.9	6
246	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into Phenix. *Acta Crystallographica Section D: Structural Biology*, **2020**, 76, 51-62	5.5	16
245	Coupled intra- and interdomain dynamics support domain cross-talk in Pin1. *Journal of Biological Chemistry*, **2020**, 295, 16585-16603	5.4	2
244	Solution NMR readily reveals distinct structural folds and interactions in doubly C- and F-labeled RNAs. *Science Advances*, **2020**, 6,	14.3	11
243	Atomistic Simulations of Heme Dissociation Pathways in Human Methemoglobins Reveal Hidden Intermediates. *Biochemistry*, **2020**, 59, 4093-4107	3.2	3
242	Rapid and accurate determination of atomistic RNA dynamic ensemble models using NMR and structure prediction. *Nature Communications*, **2020**, 11, 5531	17.4	15
241	A twist in the road less traveled: The AMBER ff15ipq-m force field for protein mimetics. *Journal of Chemical Physics*, **2020**, 153, 064101	3.9	5
240	Using quantum chemistry to estimate chemical shifts in biomolecules. *Biophysical Chemistry*, **2020**, 267, 106476	3.5	4
239	Structural basis for transcriptional start site control of HIV-1 RNA fate. *Science*, **2020**, 368, 413-417	33.3	34
238	Predicting Site-Binding Modes of Ions and Water to Nucleic Acids Using Molecular Solvation Theory. *Journal of the American Chemical Society*, **2019**, 141, 2435-2445	16.4	27

237	Molecular underpinnings of integrin binding to collagen-mimetic peptides containing vascular Ehlers-Danlos syndrome-associated substitutions. *Journal of Biological Chemistry*, **2019**, 294, 14442-14453	5.4	1
236	High-Resolution ENDOR Spectroscopy Combined with Quantum Chemical Calculations Reveals the Structure of Nitrogenase Janus Intermediate E(4H). *Journal of the American Chemical Society*, **2019**, 141, 11984-11996	16.4	33
235	Generalized Born Implicit Solvent Models for Biomolecules. *Annual Review of Biophysics*, **2019**, 48, 275-296	20.1	68
234	Characterizing Watson-Crick versus Hoogsteen Base Pairing in a DNA-Protein Complex Using Nuclear Magnetic Resonance and Site-Specifically C- and N-Labeled DNA. *Biochemistry*, **2019**, 58, 1963-1974	3.2	11
233	A molecular reconstruction approach to site-based 3D-RISM and comparison to GIST hydration thermodynamic maps in an enzyme active site. *PLoS ONE*, **2019**, 14, e0219473	3.7	16
232	Molecular Dynamics Simulations of Macromolecular Crystals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1402	7.9	9
231	Determination of accurate backbone chemical shift tensors in microcrystalline proteins by integrating MAS NMR and QM/MM. *Physical Chemistry Chemical Physics*, **2018**, 20, 9543-9553	3.6	6
230	Chemical Shifts of the Carbohydrate Binding Domain of Galectin-3 from Magic Angle Spinning NMR and Hybrid Quantum Mechanics/Molecular Mechanics Calculations. *Journal of Physical Chemistry B*, **2018**, 122, 2931-2939	3.4	5
229	Atomic structures of excited state A-T Hoogsteen base pairs in duplex DNA by combining NMR relaxation dispersion, mutagenesis, and chemical shift calculations. *Journal of Biomolecular NMR*, **2018**, 70, 229-244	3	21
228	Structure of the 30 kDa HIV-1 RNA Dimerization Signal by a Hybrid Cryo-EM, NMR, and Molecular Dynamics Approach. *Structure*, **2018**, 26, 490-498.e3	5.2	43
227	NGLview-interactive molecular graphics for Jupyter notebooks. *Bioinformatics*, **2018**, 34, 1241-1242	7.2	56
226	Reconciling Structural and Spectroscopic Fingerprints of the Oxygen-Evolving Complex of Photosystem II: A Computational Study of the S State. *Journal of Physical Chemistry B*, **2018**, 122, 11868-11882	3.4	10
225	Cryptic binding sites become accessible through surface reconstruction of the type I collagen fibril. *Scientific Reports*, **2018**, 8, 16646	4.9	16
224	Systematic Comparison of Amber and Rosetta Energy Functions for Protein Structure Evaluation. *Journal of Chemical Theory and Computation*, **2018**, 14, 6015-6025	6.4	13
223	Resolving Ambiguous Protonation and Oxidation States in the Oxygen Evolving Complex of Photosystem II. *Journal of Physical Chemistry B*, **2018**, 122, 8654-8664	3.4	13
222	GPU-Accelerated Molecular Dynamics and Free Energy Methods in Amber18: Performance Enhancements and New Features. *Journal of Chemical Information and Modeling*, **2018**, 58, 2043-2050	6.1	165
221	Propagated Perturbations from a Peripheral Mutation Show Interactions Supporting WW Domain Thermostability. *Structure*, **2018**, 26, 1474-1485.e5	5.2	9
220	Enhanced Sampling of Interdomain Motion Using Map-Restrained Langevin Dynamics and NMR: Application to Pin1. *Journal of Molecular Biology*, **2018**, 430, 2164-2180	6.5	7

219	Links between the charge model and bonded parameter force constants in biomolecular force fields. *Journal of Chemical Physics*, **2017**, 147, 161730	3.9	3
218	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 147-161	4.2	81
217	Revealing Accessibility of Cryptic Protein Binding Sites within the Functional Collagen Fibril. *Biomolecules*, **2017**, 7,	5.9	17
216	Further along the Road Less Traveled: AMBER ff15ipq, an Original Protein Force Field Built on a Self-Consistent Physical Model. *Journal of Chemical Theory and Computation*, **2016**, 12, 3926-47	6.4	108
215	Interview with David A. Case: On force fields, biomolecular modeling, and NMR. *Concepts in Magnetic Resonance Part A: Bridging Education and Research*, **2016**, 45A, e21403	0.6	
214	The Dependence of Carbohydrate-Aromatic Interaction Strengths on the Structure of the Carbohydrate. *Journal of the American Chemical Society*, **2016**, 138, 7636-48	16.4	38
213	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. *Journal of Chemical Theory and Computation*, **2016**, 12, 405-13	6.4	1303
212	Parmbsc1: a refined force field for DNA simulations. *Nature Methods*, **2016**, 13, 55-8	21.6	483
211	Extracting water and ion distributions from solution x-ray scattering experiments. *Journal of Chemical Physics*, **2016**, 144, 214105	3.9	14
210	Molecular dynamics simulation of triclinic lysozyme in a crystal lattice. *Protein Science*, **2016**, 25, 87-102	6.3	29
209	HIV-1 Capsid Function Is Regulated by Dynamics: Quantitative Atomic-Resolution Insights by Integrating Magic-Angle-Spinning NMR, QM/MM, and MD. *Journal of the American Chemical Society*, **2016**, 138, 14066-14075	16.4	40
208	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and Schrödinger FEP. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 533-9	4.2	15
207	Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 9811-32	3.4	66
206	DOCK 6: Impact of new features and current docking performance. *Journal of Computational Chemistry*, **2015**, 36, 1132-56	3.5	405
205	Modulating RNA Alignment Using Directional Dynamic Kinks: Application in Determining an Atomic-Resolution Ensemble for a Hairpin using NMR Residual Dipolar Couplings. *Journal of the American Chemical Society*, **2015**, 137, 12954-65	16.4	21
204	AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules. *Journal of Biomolecular NMR*, **2015**, 63, 125-39	3	36
203	Dynamic Water-Mediated Hydrogen Bonding in a Collagen Model Peptide. *Biochemistry*, **2015**, 54, 6029-37	3.2	18
202	Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin. *Rna*, **2015**, 21, 963-74	5.8	24

201	RNA structure. Structure of the HIV-1 RNA packaging signal. *Science*, **2015**, 348, 917-21	33.3	166
200	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. *Nature Structural and Molecular Biology*, **2015**, 22, 433-4	17.6	26
199	Competitive interaction of monovalent cations with DNA from 3D-RISM. *Nucleic Acids Research*, **2015**, 43, 8405-15	20.1	32
198	All-atom crystal simulations of DNA and RNA duplexes. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 1059-1071	4	17
197	ff14ipq: A Self-Consistent Force Field for Condensed-Phase Simulations of Proteins. *Journal of Chemical Theory and Computation*, **2014**, 10, 4515-4534	6.4	67
196	Ion counting from explicit-solvent simulations and 3D-RISM. *Biophysical Journal*, **2014**, 106, 883-94	2.9	77
195	ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucleic Acids Research*, **2014**, 42, 12272-83	20.1	138
194	Twenty-five years of nucleic acid simulations. *Biopolymers*, **2013**, 99, 969-77	2.2	124
193	Derivation of fixed partial charges for amino acids accommodating a specific water model and implicit polarization. *Journal of Physical Chemistry B*, **2013**, 117, 2328-38	3.4	79
192	Targeted conformational search with map-restrained self-guided Langevin dynamics: application to flexible fitting into electron microscopic density maps. *Journal of Structural Biology*, **2013**, 183, 429-440	3.4	35
191	Characterization of [4Fe-4S] cluster vibrations and structure in nitrogenase Fe protein at three oxidation levels via combined NRVS, EXAFS, and DFT analyses. *Journal of the American Chemical Society*, **2013**, 135, 2530-43	16.4	38
190	Chemical shifts in biomolecules. *Current Opinion in Structural Biology*, **2013**, 23, 172-6	8.1	36
189	An overview of the Amber biomolecular simulation package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 198-210	7.9	1187
188	Simple electrolyte solutions: comparison of DRISM and molecular dynamics results for alkali halide solutions. *Journal of Chemical Physics*, **2013**, 138, 044103	3.9	53
187	Peptide crystal simulations reveal hidden dynamics. *Journal of the American Chemical Society*, **2013**, 135, 7938-48	16.4	28
186	Free energy calculations on the binding of novel thiolactomycin derivatives to E. coli fatty acid synthase I. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 3446-53	3.4	8
185	Sucrose in aqueous solution revisited, Part 2: adaptively biased molecular dynamics simulations and computational analysis of NMR relaxation. *Biopolymers*, **2012**, 97, 289-302	2.2	11
184	Sucrose in aqueous solution revisited, Part 1: molecular dynamics simulations and direct and indirect dipolar coupling analysis. *Biopolymers*, **2012**, 97, 276-88	2.2	23

183	Implicit Solvent Models and Electrostatics in Molecular Recognition **2012**, 171-189		
182	Chapter 4:Integral Equation Theory of Biomolecules and Electrolytes. *RSC Biomolecular Sciences*, **2012**, 51-86		12
181	Energetic selection of topology in ferredoxins. *PLoS Computational Biology*, **2012**, 8, e1002463	5	26
180	Searching and optimizing structure ensembles for complex flexible sugars. *Journal of the American Chemical Society*, **2011**, 133, 15252-5	16.4	18
179	Comparison of SARS and NL63 papain-like protease binding sites and binding site dynamics: inhibitor design implications. *Journal of Molecular Biology*, **2011**, 414, 272-88	6.5	17
178	Evaluation of DNA Force Fields in Implicit Solvation. *Journal of Chemical Theory and Computation*, **2011**, 7, 3181-3198	6.4	34
177	Calculation of chemical shift anisotropy in proteins. *Journal of Biomolecular NMR*, **2011**, 51, 303-12	3	38
176	In Silico: An Alternate Approach to Chemistry and Biology **2011**, 19-31		
175	Soft-core potentials in thermodynamic integration: comparing one- and two-step transformations. *Journal of Computational Chemistry*, **2011**, 32, 3253-63	3.5	137
174	Fe-H/D stretching and bending modes in nuclear resonant vibrational, Raman and infrared spectroscopies: comparisons of density functional theory and experiment. *Faraday Discussions*, **2011**, 148, 409-20; discussion 421-41	3.6	27
173	Multi-Level Ewald: A hybrid multigrid / Fast Fourier Transform approach to the electrostatic particle-mesh problem. *Journal of Chemical Theory and Computation*, **2010**, 6, 443-58	6.4	24
172	Three-dimensional molecular theory of solvation coupled with molecular dynamics in Amber. *Journal of Chemical Theory and Computation*, **2010**, 6, 607-624	6.4	197
171	Simulations of a protein crystal with a high resolution X-ray structure: evaluation of force fields and water models. *Journal of Physical Chemistry B*, **2010**, 114, 12811-24	3.4	61
170	A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA. *Nucleic Acids Research*, **2010**, 38, 299-313	20.1	299
169	The Ornstein–Zernike equation in molecular electronic structure theory. *Molecular Physics*, **2010**, 108, 307-314	1.7	7
168	Proton Transfer Studied Using a Combined Ab Initio Reactive Potential Energy Surface with Quantum Path Integral Methodology. *Journal of Chemical Theory and Computation*, **2010**, 6, 2566-2580	6.4	41
167	Major groove width variations in RNA structures determined by NMR and impact of 13C residual chemical shift anisotropy and 1H-13C residual dipolar coupling on refinement. *Journal of Biomolecular NMR*, **2010**, 47, 205-19	3	60
166	Influence of the coupling of interdomain and overall motions on NMR relaxation. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 11016-21	11.5	42

165	Characterization of domain-peptide interaction interface: a generic structure-based model to decipher the binding specificity of SH3 domains. *Molecular and Cellular Proteomics*, **2009**, 8, 639-49	7.6	92
164	Evaluating beta-turn mimics as beta-sheet folding nucleators. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 11067-72	11.5	84
163	DOCK 6: combining techniques to model RNA-small molecule complexes. *Rna*, **2009**, 15, 1219-30	5.8	510
162	Water-induced polaron formation at the pentacene surface: Quantum mechanical molecular mechanics simulations. *Physical Review B*, **2009**, 79,	3.3	42
161	Quantum dynamical effects in liquid water: A semiclassical study on the diffusion and the infrared absorption spectrum. *Journal of Chemical Physics*, **2009**, 131, 164509	3.9	69
160	Evaluating rotational diffusion from protein MD simulations. *Journal of Physical Chemistry B*, **2008**, 112, 6013-24	3.4	114
159	Direct simulation of electron transfer reactions in DNA radical cations. *Journal of Physical Chemistry B*, **2008**, 112, 16935-44	3.4	50
158	Characterization of domain-peptide interaction interface: a case study on the amphiphysin-1 SH3 domain. *Journal of Molecular Biology*, **2008**, 376, 1201-14	6.5	179
157	Rescoring docking hit lists for model cavity sites: predictions and experimental testing. *Journal of Molecular Biology*, **2008**, 377, 914-34	6.5	149
156	Characterization of the Fe site in iron-sulfur cluster-free hydrogenase (Hmd) and of a model compound via nuclear resonance vibrational spectroscopy (NRVS). *Inorganic Chemistry*, **2008**, 47, 3969-77	5.1	88
155	Carbon-deuterium bonds as probes of dihydrofolate reductase. *Journal of the American Chemical Society*, **2008**, 130, 6597-603	16.4	51
154	Toward a chemical mechanism of proton pumping by the B-type cytochrome c oxidases: application of density functional theory to cytochrome ba3 of Thermus thermophilus. *Journal of the American Chemical Society*, **2008**, 130, 15002-21	16.4	60
153	Ligand-bound S = 1/2 FeMo-cofactor of nitrogenase: hyperfine interaction analysis and implication for the central ligand X identity. *Inorganic Chemistry*, **2008**, 47, 6162-72	5.1	51
152	DNA oligonucleotides with A, T, G or C opposite an abasic site: structure and dynamics. *Nucleic Acids Research*, **2008**, 36, 253-62	20.1	54
151	The implementation of a fast and accurate QM/MM potential method in Amber. *Journal of Computational Chemistry*, **2008**, 29, 1019-31	3.5	289
150	Multiscale modeling of nucleic acids: insights into DNA flexibility. *Biopolymers*, **2008**, 89, 722-31	2.2	29
149	Extended sugar-assisted glycopeptide ligations: development, scope, and applications. *Journal of the American Chemical Society*, **2007**, 129, 13527-36	16.4	82
148	Testing if the interstitial atom, X, of the nitrogenase molybdenum-iron cofactor is N or C: ENDOR, ESEEM, and DFT studies of the S = 3/2 resting state in multiple environments. *Inorganic Chemistry*, **2007**, 46, 11437-49	5.1	77

147	Generalized Born model with a simple, robust molecular volume correction. *Journal of Chemical Theory and Computation*, **2007**, 3, 156-169	6.4	267
146	Implementation of the SCC-DFTB method for hybrid QM/MM simulations within the amber molecular dynamics package. *Journal of Physical Chemistry A*, **2007**, 111, 5655-64	2.8	183
145	A new model for chemical shifts of amide hydrogens in proteins. *Journal of Biomolecular NMR*, **2007** , 38, 139-50	3	53
144	Vibrational averaging of chemical shift anisotropies in model peptides. *Journal of Biomolecular NMR*, **2007**, 38, 255-66	3	27
143	Nonlinear scaling schemes for Lennard-Jones interactions in free energy calculations. *Journal of Chemical Physics*, **2007**, 127, 214108	3.9	240
142	Automatic atom type and bond type perception in molecular mechanical calculations. *Journal of Molecular Graphics and Modelling*, **2006**, 25, 247-60	2.8	3191
141	A comparison of quantum chemical models for calculating NMR shielding parameters in peptides: mixed basis set and ONIOM methods combined with a complete basis set extrapolation. *Journal of Computational Chemistry*, **2006**, 27, 825-36	3.5	61
140	Second derivatives in generalized Born theory. *Journal of Computational Chemistry*, **2006**, 27, 1662-75	3.5	26
139	An accurate and simple quantum model for liquid water. *Journal of Chemical Physics*, **2006**, 125, 184507	3.9	165
138	A multistep approach to structure-based drug design: studying ligand binding at the human neutrophil elastase. *Journal of Medicinal Chemistry*, **2006**, 49, 1837-44	8.3	73
137	Low-Resolution Molecular Dynamics Simulations of the 30S Ribosomal Subunit. *Multiscale Modeling and Simulation*, **2006**, 5, 1248-1263	1.8	14
136	Estimation of Absolute Free Energies of Hydration Using Continuum Methods: Accuracy of Partial Charge Models and Optimization of Nonpolar Contributions. *Journal of Chemical Theory and Computation*, **2006**, 2, 128-39	6.4	143
135	How nitrogenase shakes--initial information about P-cluster and FeMo-cofactor normal modes from nuclear resonance vibrational spectroscopy (NRVS). *Journal of the American Chemical Society*, **2006**, 128, 7608-12	16.4	67
134	Induced fit and "lock and key" recognition of 5S RNA by zinc fingers of transcription factor IIIA. *Journal of Molecular Biology*, **2006**, 357, 275-91	6.5	60
133	Nudged elastic band calculation of minimal energy paths for the conformational change of a GG non-canonical pair. *Journal of Molecular Biology*, **2006**, 357, 1683-93	6.5	37
132	Molecular dynamics simulations of the 136 unique tetranucleotide sequences of DNA oligonucleotides. II: sequence context effects on the dynamical structures of the 10 unique dinucleotide steps. *Biophysical Journal*, **2005**, 89, 3721-40	2.9	187
131	Differential solvation and tautomer stability of a model base pair within the minor and major grooves of DNA. *Journal of the American Chemical Society*, **2005**, 127, 15612-7	16.4	52
130	Biomolecular simulations at constant pH. *Current Opinion in Structural Biology*, **2005**, 15, 157-63	8.1	126

129	The Amber biomolecular simulation programs. *Journal of Computational Chemistry*, **2005**, 26, 1668-88	3.5	6155
128	NMR structure of a cyclic polyamide-DNA complex. *Journal of the American Chemical Society*, **2004**, 126, 7958-66	16.4	37
127	Exploring protein native states and large-scale conformational changes with a modified generalized born model. *Proteins: Structure, Function and Bioinformatics*, **2004**, 55, 383-94	4.2	1728
126	Change in protein flexibility upon complex formation: analysis of Ras-Raf using molecular dynamics and a molecular framework approach. *Proteins: Structure, Function and Bioinformatics*, **2004**, 56, 322-37	4.2	94
125	Predicting interactions of winged-helix transcription factors with DNA. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 172-87	4.2	19
124	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. *Journal of Computational Chemistry*, **2004**, 25, 265-84	3.5	465
123	Converging free energy estimates: MM-PB(GB)SA studies on the protein-protein complex Ras-Raf. *Journal of Computational Chemistry*, **2004**, 25, 238-50	3.5	652
122	Development and testing of a general amber force field. *Journal of Computational Chemistry*, **2004**, 25, 1157-74	3.5	10682
121	Constant pH molecular dynamics in generalized Born implicit solvent. *Journal of Computational Chemistry*, **2004**, 25, 2038-48	3.5	368
120	Proton binding to proteins: pK(a) calculations with explicit and implicit solvent models. *Journal of the American Chemical Society*, **2004**, 126, 4167-80	16.4	239
119	Molecular dynamics simulations of the 136 unique tetranucleotide sequences of DNA oligonucleotides. I. Research design and results on d(CpG) steps. *Biophysical Journal*, **2004**, 87, 3799-813	2.9	223
118	NMR Parameters in Proteins and Nucleic Acids **2004**, 339-351		1
117	A novel method for finding tRNA genes. *Rna*, **2003**, 9, 507-17	5.8	12
116	Design and synthesis of highly constrained factor Xa inhibitors: amidine-substituted bis(benzoyl)--diazepan-2-ones and bis(benzylidene)-bis(gem-dimethyl)cycloketones. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 3379-92	3.4	13
115	Reintroducing electrostatics into protein X-ray structure refinement: bulk solvent treated as a dielectric continuum. *Acta Crystallographica Section D: Biological Crystallography*, **2003**, 59, 2094-103		29
114	Force fields for protein simulations. *Advances in Protein Chemistry*, **2003**, 66, 27-85		1303
113	Density functional and reduction potential calculations of Fe4S4 clusters. *Journal of the American Chemical Society*, **2003**, 125, 1923-36	16.4	189
112	The circumsphere as a tool to assess distortion in [4Fe-4S] atom clusters. *Journal of Biological Inorganic Chemistry*, **2003**, 8, 519-526	3.7	18

111	Structural, spectroscopic, and redox consequences of a central ligand in the FeMoco of nitrogenase: a density functional theoretical study. *Journal of the American Chemical Society*, **2003**, 125, 8377-83	16.4	133
110	Insights into the mobility of methyl-bearing side chains in proteins from (3)J(CC) and (3)J(CN) couplings. *Journal of the American Chemical Society*, **2003**, 125, 8959-66	16.4	114
109	Structural details, pathways, and energetics of unfolding apomyoglobin. *Journal of Molecular Biology*, **2003**, 325, 555-67	6.5	50
108	Modeling of flap endonuclease interactions with DNA substrate. *Journal of Molecular Biology*, **2003**, 328, 537-54	6.5	34
107	Insights into protein-protein binding by binding free energy calculation and free energy decomposition for the Ras-Raf and Ras-RalGDS complexes. *Journal of Molecular Biology*, **2003**, 330, 891-913	6.5	924
106	Symmetry and bonding in metalloporphyrins. A modern implementation for the bonding analyses of five- and six-coordinate high-spin iron(III)-porphyrin complexes through density functional calculation and NMR spectroscopy. *Journal of the American Chemical Society*, **2003**, 125, 6774-83	16.4	70
105	Drug-Target Binding Forces: Advances in Force Field Approaches **2003**, 169-185		1
104	RNAML: a standard syntax for exchanging RNA information. *Rna*, **2002**, 8, 707-17	5.8	68
103	Effective Born radii in the generalized Born approximation: the importance of being perfect. *Journal of Computational Chemistry*, **2002**, 23, 1297-304	3.5	364
102	Density functional calculation of p K(a) values and redox potentials in the bovine Rieske iron-sulfur protein. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 632-9	3.7	103
101	FeMo cofactor of nitrogenase: energetics and local interactions in the protein environment. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 735-49	3.7	40
100	Comparison of protein solution structures refined by molecular dynamics simulation in vacuum, with a generalized Born model, and with explicit water. *Journal of Biomolecular NMR*, **2002**, 22, 317-31	3	105
99	Binding modes for the first coupled electron and proton addition to FeMoco of nitrogenase. *Journal of the American Chemical Society*, **2002**, 124, 4546-7	16.4	40
98	Flexibility of an Antibody Binding Site Measured with Photon Echo Spectroscopy. *Journal of Physical Chemistry B*, **2002**, 106, 1090-1103	3.4	41
97	Metal substitution in the active site of nitrogenase MFe(7)S(9) (M = Mo(4+), V(3+), Fe(3+)). *Inorganic Chemistry*, **2002**, 41, 5744-53	5.1	48
96	Molecular dynamics and NMR spin relaxation in proteins. *Accounts of Chemical Research*, **2002**, 35, 325-31	14.3	177
95	Automated prediction of 15N, 13Calpha, 13Cbeta and 13C' chemical shifts in proteins using a density functional database. *Journal of Biomolecular NMR*, **2001**, 21, 321-33	3	240
94	Continuum solvent molecular dynamics study of flexibility in interleukin-8. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 136-45	2.8	24

93	Vectorization of the generalized Born model for molecular dynamics on shared-memory computers. *Computational and Theoretical Chemistry*, **2001**, 549, 193-201		6
92	Optimized particle-mesh Ewald/multiple-time step integration for molecular dynamics simulations. *Journal of Chemical Physics*, **2001**, 115, 4003-4018	3.9	162
91	Calculations of the Absolute Free Energies of Binding between RNA and Metal Ions Using Molecular Dynamics Simulations and Continuum Electrostatics. *Journal of Physical Chemistry B*, **2001**, 105, 11314-11325	3.4	70
90	Solution structure and dynamics of yeast elongin C in complex with a von Hippel-Lindau peptide. *Journal of Molecular Biology*, **2001**, 312, 177-86	6.5	25
89	RNAMotif, an RNA secondary structure definition and search algorithm. *Nucleic Acids Research*, **2001**, 29, 4724-35	20.1	338
88	FeMo cofactor of nitrogenase: a density functional study of states M(N), M(OX), M(R), and M(I). *Journal of the American Chemical Society*, **2001**, 123, 12392-410	16.4	152
87	Theory and applications of the generalized Born solvation model in macromolecular simulations. *Biopolymers*, **2000**, 56, 275-91	2.2	787
86	Assessment of zinc finger orientations by residual dipolar coupling constants. *Journal of Biomolecular NMR*, **2000**, 16, 9-21	3	40
85	Calculating structures and free energies of complex molecules: combining molecular mechanics and continuum models. *Accounts of Chemical Research*, **2000**, 33, 889-97	24.3	3346
84	Generalized born models of macromolecular solvation effects. *Annual Review of Physical Chemistry*, **2000**, 51, 129-52	15.7	977
83	Perspective on Dynamics of folded proteins. *Theoretical Chemistry Accounts*, **2000**, 103, 332-334	1.9	
82	NMR solution structure of the inserted domain of human leukocyte function associated antigen-1. *Journal of Molecular Biology*, **2000**, 295, 1251-64	6.5	65
81	The structural basis for in situ activation of DNA alkylation by duocarmycin SA. *Journal of Molecular Biology*, **2000**, 300, 1195-204	6.5	25
80	NMR and molecular dynamics studies of the hydration of a zinc finger-DNA complex. *Journal of Molecular Biology*, **2000**, 302, 1101-17	6.5	47
79	A Phototautomerizable Model DNA Base Pair. *Journal of the American Chemical Society*, **2000**, 122, 9917-9920	16.4	71
78	Modification of the Generalized Born Model Suitable for Macromolecules. *Journal of Physical Chemistry B*, **2000**, 104, 3712-3720	3.4	830
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