David A Case

List of Publications by Citations

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	Development and testing of a general amber force field. *Journal of Computational Chemistry*, **2004**, 25, 1157-74	3.5	10682
253	The Amber biomolecular simulation programs. *Journal of Computational Chemistry*, **2005**, 26, 1668-88	3.5	6155
252	A new force field for molecular mechanical simulation of nucleic acids and proteins. *Journal of the American Chemical Society*, **1984**, 106, 765-784	16.4	4364
251	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
250	Automatic atom type and bond type perception in molecular mechanical calculations. *Journal of Molecular Graphics and Modelling*, **2006**, 25, 247-60	2.8	3191
249	An all atom force field for simulations of proteins and nucleic acids. *Journal of Computational Chemistry*, **1986**, 7, 230-252	3.5	2957
248	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
247	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
246	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
245	Force fields for protein simulations. *Advances in Protein Chemistry*, **2003**, 66, 27-85		1303
244	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidate□DNA Helices. *Journal of the American Chemical Society*, **1998**, 120, 9401-9409	16.4	1269
243	An overview of the Amber biomolecular simulation package. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 198-210	7.9	1187
242	Generalized born models of macromolecular solvation effects. *Annual Review of Physical Chemistry*, **2000**, 51, 129-52	15.7	977
241	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
240	Modification of the Generalized Born Model Suitable for Macromolecules. *Journal of Physical Chemistry B*, **2000**, 104, 3712-3720	3.4	830
239	Theory and applications of the generalized Born solvation model in macromolecular simulations. *Biopolymers*, **2000**, 56, 275-91	2.2	787
238	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

237	Structural basis for DNA bending by the architectural transcription factor LEF-1. *Nature*, **1995**, 376, 791-5	50.4	524
236	Density-Functional Theory of Spin Polarization and Spin Coupling in Iron Sulfur Clusters. *Advances in Inorganic Chemistry*, **1992**, 38, 423-470	2.1	513
235	DOCK 6: combining techniques to model RNA-small molecule complexes. *Rna*, **2009**, 15, 1219-30	5.8	510
234	Parmbsc1: a refined force field for DNA simulations. *Nature Methods*, **2016**, 13, 55-8	21.6	483
233	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
232	DOCK 6: Impact of new features and current docking performance. *Journal of Computational Chemistry*, **2015**, 36, 1132-56	3.5	405
231	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. *Journal of the American Chemical Society*, **2000**, 122, 2489-2498	16.4	374
230	Constant pH molecular dynamics in generalized Born implicit solvent. *Journal of Computational Chemistry*, **2004**, 25, 2038-48	3.5	368
229	Effective Born radii in the generalized Born approximation: the importance of being perfect. *Journal of Computational Chemistry*, **2002**, 23, 1297-304	3.5	364
228	RNAMotif, an RNA secondary structure definition and search algorithm. *Nucleic Acids Research*, **2001**, 29, 4724-35	20.1	338
227	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
226	The implementation of a fast and accurate QM/MM potential method in Amber. *Journal of Computational Chemistry*, **2008**, 29, 1019-31	3.5	289
225	Models for ferredoxins: electronic structures of iron-sulfur clusters with one, two, and four iron atoms. *Journal of the American Chemical Society*, **1985**, 107, 3418-3426	16.4	274
224	Density Functional/Poisson-Boltzmann Calculations of Redox Potentials for Iron-Sulfur Clusters. *Journal of the American Chemical Society*, **1994**, 116, 11898-11914	16.4	272
223	Generalized Born model with a simple, robust molecular volume correction. *Journal of Chemical Theory and Computation*, **2007**, 3, 156-169	6.4	267
222	High-resolution solution structures of oxidized and reduced Escherichia coli thioredoxin. *Structure*, **1994**, 2, 853-68	5.2	267
221	A new analysis of proton chemical shifts in proteins. *Journal of the American Chemical Society*, **1991**, 113, 9436-9444	16.4	267
220	Application of a pairwise generalized Born model to proteins and nucleic acids: inclusion of salt effects. *Theoretical Chemistry Accounts*, **1999**, 101, 426-434	1.9	244

219	Nonlinear scaling schemes for Lennard-Jones interactions in free energy calculations. *Journal of Chemical Physics*, **2007**, 127, 214108	3.9	240
218	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
217	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
216	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
215	Simulations of peptide conformational dynamics and thermodynamics. *Chemical Reviews*, **1993**, 93, 2487-502	62.0	205
214	Broken symmetry analysis of spin coupling in iron-sulfur clusters. *Journal of the American Chemical Society*, **1988**, 110, 1001-1005	16.4	204
213	Electronic structure of Ru2(O2CR)4+ and Rh2(O2CR)4+ complexes. *Journal of the American Chemical Society*, **1979**, 101, 5256-5267	16.4	204
212	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
211	Density functional and reduction potential calculations of Fe4S4 clusters. *Journal of the American Chemical Society*, **2003**, 125, 1923-36	16.4	189
210	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
209	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
208	Continuum solvent studies of the stability of RNA hairpin loops and helices. *Journal of Biomolecular Structure and Dynamics*, **1998**, 16, 671-82	3.6	180
207	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
206	Molecular dynamics and NMR spin relaxation in proteins. *Accounts of Chemical Research*, **2002**, 35, 325-31	14.3	177
205	Solution structure of the first three zinc fingers of TFIIIA bound to the cognate DNA sequence: determinants of affinity and sequence specificity. *Journal of Molecular Biology*, **1997**, 273, 183-206	6.5	171
204	RNA structure. Structure of the HIV-1 RNA packaging signal. *Science*, **2015**, 348, 917-21	33.3	166
203	An accurate and simple quantum model for liquid water. *Journal of Chemical Physics*, **2006**, 125, 184507	3.9	165
202	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

201	Molecular dynamics and continuum solvent studies of the stability of polyG-polyC and polyA-polyT DNA duplexes in solution. *Journal of Biomolecular Structure and Dynamics*, **1998**, 16, 265-80	3.6	163
200	Optimized particle-mesh Ewald/multiple-time step integration for molecular dynamics simulations. *Journal of Chemical Physics*, **2001**, 115, 4003-4018	3.9	162
199	The structure of calcyclin reveals a novel homodimeric fold for S100 Ca(2+)-binding proteins. *Nature Structural and Molecular Biology*, **1995**, 2, 790-6	17.6	158
198	Incorporating Solvation Effects into Density Functional Electronic Structure Calculations. *The Journal of Physical Chemistry*, **1994**, 98, 11059-11068		158
197	Dynamics of ligand escape from the heme pocket of myoglobin. *Journal of the American Chemical Society*, **1988**, 110, 7690-7697	16.4	156
196	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
195	Theories of chemical shift anisotropies in proteins and nucleic acids. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **1998**, 32, 165-190	10.4	151
194	Rescoring docking hit lists for model cavity sites: predictions and experimental testing. *Journal of Molecular Biology*, **2008**, 377, 914-34	6.5	149
193	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
192	ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. *Nucleic Acids Research*, **2014**, 42, 12272-83	20.1	138
191	Soft-core potentials in thermodynamic integration: comparing one- and two-step transformations. *Journal of Computational Chemistry*, **2011**, 32, 3253-63	3.5	137
190	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
189	Unfolding of an alpha-helix in water. *Biopolymers*, **1991**, 31, 1351-61	2.2	130
188	Biomolecular simulations at constant pH. *Current Opinion in Structural Biology*, **2005**, 15, 157-63	8.1	126
187	Twenty-five years of nucleic acid simulations. *Biopolymers*, **2013**, 99, 969-77	2.2	124
186	Evaluating rotational diffusion from protein MD simulations. *Journal of Physical Chemistry B*, **2008**, 112, 6013-24	3.4	114
185	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
184	Molecular dynamics analysis of NMR relaxation in a zinc-finger peptide. *Journal of the American Chemical Society*, **1992**, 114, 9059-9067	16.4	112

183	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
182	Including Side Chain Flexibility in Continuum Electrostatic Calculations of Protein Titration. *The Journal of Physical Chemistry*, **1996**, 100, 20156-20163		106
181	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
180	High-resolution solution structure of reduced French bean plastocyanin and comparison with the crystal structure of poplar plastocyanin. *Journal of Molecular Biology*, **1991**, 221, 533-55	6.5	104
179	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
178	Domain packing and dynamics in the DNA complex of the N-terminal zinc fingers of TFIIIA. *Nature Structural Biology*, **1997**, 4, 605-8		102
177	Electronic structure calculations on active site models for 4-Fe,4-S iron-sulfur proteins. *Journal of the American Chemical Society*, **1982**, 104, 3269-3279	16.4	102
176	Use of chemical shifts and coupling constants in nuclear magnetic resonance structural studies on peptides and proteins. *Methods in Enzymology*, **1994**, 239, 392-416	1.7	99
175	Solution structure of carbonmonoxy myoglobin determined from nuclear magnetic resonance distance and chemical shift constraints. *Journal of Molecular Biology*, **1994**, 244, 183-97	6.5	97
174	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
173	The calculation of one-electron properties from X□multiple scattering wavefunctions. *Chemical Physics Letters*, **1976**, 39, 33-38	2.5	94
172	Calculations of NMR dipolar coupling strengths in model peptides. *Journal of Biomolecular NMR*, **1999**, 15, 95-102	3	93
171	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
170	Density Functional Study on the Electronic Structures of Model Peroxidase Compounds I and II. *Journal of the American Chemical Society*, **1997**, 119, 11442-11451	16.4	88
169	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
168	Xalpha multiple scattering calculations on copper porphine. *Journal of the American Chemical Society*, **1977**, 99, 6182-94	16.4	87
167	Static and Dynamic Effects on Vicinal ScalarJCouplings in Proteins and Peptides:□A MD/DFT Analysis. *Journal of the American Chemical Society*, **2000**, 122, 10390-10397	16.4	85
166	NMR solution structure of Cu(I) rusticyanin from Thiobacillus ferrooxidans: structural basis for the extreme acid stability and redox potential. *Journal of Molecular Biology*, **1996**, 263, 752-67	6.5	85

165	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
164	Extended sugar-assisted glycopeptide ligations: development, scope, and applications. *Journal of the American Chemical Society*, **2007**, 129, 13527-36	16.4	82
163	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 147-161	4.2	81
162	Density Functional Calculations of Proton Chemical Shifts in Model Peptides. *Journal of the American Chemical Society*, **1997**, 119, 12262-12273	16.4	80
161	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
160	Ion counting from explicit-solvent simulations and 3D-RISM. *Biophysical Journal*, **2014**, 106, 883-94	2.9	77
159	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
158	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
157	A Phototautomerizable Model DNA Base Pair. *Journal of the American Chemical Society*, **2000**, 122, 9917-9920	16.4	71
156	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
155	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
154	Characterization of biomolecular structure and dynamics by NMR cross relaxation. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **1994**, 26, 27-58	10.4	70
153	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
152	Generalized Born Implicit Solvent Models for Biomolecules. *Annual Review of Biophysics*, **2019**, 48, 275-296	22.1	68
151	RNAML: a standard syntax for exchanging RNA information. *Rna*, **2002**, 8, 707-17	5.8	68
150	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
149	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
148	Advanced Potential Energy Surfaces for Molecular Simulation. *Journal of Physical Chemistry B*, **2016**, 120, 9811-32	3.4	66

147	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
146	Computational methods for determining protein structures from NMR data. *Biochemical Pharmacology*, **1990**, 40, 15-22	6	62
145	Relativistic scattered wave calculations on UF6. *Journal of Chemical Physics*, **1980**, 72, 3443-3448	3.9	62
144	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
143	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
142	Nature of the iron-oxygen bond in oxyhemoglobin. *Journal of the American Chemical Society*, **1977**, 99, 6103-5	16.4	61
141	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
140	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
139	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
138	NGLview-interactive molecular graphics for Jupyter notebooks. *Bioinformatics*, **2018**, 34, 1241-1242	7.2	56
137	Density Functional Study of Ribose and Deoxyribose Chemical Shifts. *Journal of Physical Chemistry A*, **1998**, 102, 5280-5289	2.8	56
136	Application of X□multiple-scattering theory to planar organic molecules: One-electron properties and ionization potentials of benzene, pyridine, pyrazine, pyrrole, and imidazole. *Journal of Chemical Physics*, **1980**, 73, 3294-3313	3.9	56
135	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
134	Relativistic effects on molecular hyperfine interactions: Application to XeF and CsO. *Journal of Chemical Physics*, **1983**, 79, 4939-4949	3.9	54
133	Simple electrolyte solutions: comparison of DRISM and molecular dynamics results for alkali halide solutions. *Journal of Chemical Physics*, **2013**, 138, 044103	3.9	53
132	A new model for chemical shifts of amide hydrogens in proteins. *Journal of Biomolecular NMR*, **2007**, 38, 139-50	3	53
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	Dynamics of a type VI reverse turn in a linear peptide in aqueous solution. *Folding & Design*, **1997**, 2, 35-46		51

129	Carbon-deuterium bonds as probes of dihydrofolate reductase. *Journal of the American Chemical Society*, **2008**, 130, 6597-603	16.4	51
128	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
127	Direct simulation of electron transfer reactions in DNA radical cations. *Journal of Physical Chemistry B*, **2008**, 112, 16935-44	3.4	50
126	Structural details, pathways, and energetics of unfolding apomyoglobin. *Journal of Molecular Biology*, **2003**, 325, 555-67	6.5	50
125	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
124	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
123	High resolution solution structure of a DNA duplex alkylated by the antitumor agent duocarmycin SA. *Journal of Molecular Biology*, **1997**, 272, 237-52	6.5	46
122	Calculations of proton-binding thermodynamics in proteins. *Methods in Enzymology*, **1998**, 295, 170-89	1.7	46
121	Collective NMR relaxation model applied to protein dynamics. *Physical Review Letters*, **1994**, 72, 940-943	7.4	46
120	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
119	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
118	Water-induced polaron formation at the pentacene surface: Quantum mechanical molecular mechanics simulations. *Physical Review B*, **2009**, 79,	3.3	42
117	X multiple scattering calculations on iron(II) porphine. *Journal of Chemical Physics*, **1983**, 79, 2881-2892	3.9	42
116	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
115	Flexibility of an Antibody Binding Site Measured with Photon Echo Spectroscopy. *Journal of Physical Chemistry B*, **2002**, 106, 1090-1103	3.4	41
114	FeMo cofactor of nitrogenase: energetics and local interactions in the protein environment. *Journal of Biological Inorganic Chemistry*, **2002**, 7, 735-49	3.7	40
113	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
112	Assessment of zinc finger orientations by residual dipolar coupling constants. *Journal of Biomolecular NMR*, **2000**, 16, 9-21	3	40

111	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
110	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
109	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
108	Calculation of chemical shift anisotropy in proteins. *Journal of Biomolecular NMR*, **2011**, 51, 303-12	3	38
107	Thermodynamics of a reverse turn motif. Solvent effects and side-chain packing. *Journal of Molecular Biology*, **1997**, 270, 305-17	6.5	38
106	Spin-orbit and spin-polarization effects in neptunium hexafluoride. *Journal of Chemical Physics*, **1985**, 83, 5792-5796	3.9	38
105	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
104	NMR structure of a cyclic polyamide-DNA complex. *Journal of the American Chemical Society*, **2004**, 126, 7958-66	16.4	37
103	Stereochemistry of carbon monoxide binding to myoglobin and hemoglobin. *Journal of Molecular Biology*, **1978**, 123, 697-701	6.5	37
102	AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules. *Journal of Biomolecular NMR*, **2015**, 63, 125-39	3	36
101	Chemical shifts in biomolecules. *Current Opinion in Structural Biology*, **2013**, 23, 172-6	8.1	36
100	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
99	Evaluation of DNA Force Fields in Implicit Solvation. *Journal of Chemical Theory and Computation*, **2011**, 7, 3181-3198	6.4	34
98	Modeling of flap endonuclease interactions with DNA substrate. *Journal of Molecular Biology*, **2003**, 328, 537-54	6.5	34
97	Structural basis for transcriptional start site control of HIV-1 RNA fate. *Science*, **2020**, 368, 413-417	33.3	34
96	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
95	Competitive interaction of monovalent cations with DNA from 3D-RISM. *Nucleic Acids Research*, **2015**, 43, 8405-15	20.1	32
94	Density-functional calculations of spin coupling in [Fe4S4]3+ clusters. *International Journal of Quantum Chemistry*, **1995**, 56, 95-102	2.1	31

93	Multiscale modeling of nucleic acids: insights into DNA flexibility. *Biopolymers*, **2008**, 89, 722-31	2.2	29
92	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
91	Molecular dynamics simulation of triclinic lysozyme in a crystal lattice. *Protein Science*, **2016**, 25, 87-102	6.3	29
90	Peptide crystal simulations reveal hidden dynamics. *Journal of the American Chemical Society*, **2013**, 135, 7938-48	16.4	28
89	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
88	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
87	A Computational Study of the Role of Solvation Effects in Reverse Turn Formation in the Tetrapeptides APGD and APGN. *Journal of the American Chemical Society*, **1997**, 119, 4964-4971	16.4	27
86	Vibrational averaging of chemical shift anisotropies in model peptides. *Journal of Biomolecular NMR*, **2007**, 38, 255-66	3	27
85	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
84	Energetic selection of topology in ferredoxins. *PLoS Computational Biology*, **2012**, 8, e1002463	5	26
83	Second derivatives in generalized Born theory. *Journal of Computational Chemistry*, **2006**, 27, 1662-75	3.5	26
82	Large Variations in One-Bond 13C□3C□ Couplings in Polypeptides Correlate with Backbone Conformation. *Journal of the American Chemical Society*, **2000**, 122, 2168-2171	16.4	26
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	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
79	Dynamic simulations of oxygen binding to myoglobin. *Annals of the New York Academy of Sciences*, **1986**, 482, 222-33	6.5	25
78	Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin. *Rna*, **2015**, 21, 963-74	5.8	24
77	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
76	Continuum solvent molecular dynamics study of flexibility in interleukin-8. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 136-45	2.8	24

75	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
74	Molecular dynamics analysis of a ribonuclease C-peptide analogue. *Biopolymers*, **1993**, 33, 1567-80	2.2	22
73	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
72	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
71	Molecular Dynamics Docking Driven by NMR-Derived Restraints to Determine the Structure of the Calicheamicin 1I Oligosaccharide Domain Complexed to Duplex DNA. *Magnetic Resonance in Chemistry*, **1996**, 34, S147-S155	2.1	20
70	Predicting interactions of winged-helix transcription factors with DNA. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 172-87	4.2	19
69	Dynamic Water-Mediated Hydrogen Bonding in a Collagen Model Peptide. *Biochemistry*, **2015**, 54, 6029-37	3.2	18
68	Searching and optimizing structure ensembles for complex flexible sugars. *Journal of the American Chemical Society*, **2011**, 133, 15252-5	16.4	18
67	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
66	A combined 2D-NMR and molecular dynamics analysis of the structure of the actinomycin D: d(ATGCAT)2 complex. *Journal of Biomolecular Structure and Dynamics*, **1989**, 6, 929-69	3.6	18
65	Relativistic scattered wave calculations of hexachloro- and hexabromoiridate (IV). *Journal of Chemical Physics*, **1984**, 81, 4554-4563	3.9	18
64	Kinetics of stereochemical rearrangements for mixed .beta.-diketonate complexes of aluminum(III). *Inorganic Chemistry*, **1971**, 10, 482-486	5.1	18
63	Revealing Accessibility of Cryptic Protein Binding Sites within the Functional Collagen Fibril. *Biomolecules*, **2017**, 7,	5.9	17
62	All-atom crystal simulations of DNA and RNA duplexes. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 1059-1071	4	17
61	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
60	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
59	Distributed torsion angle grid search in high dimensions: a systematic approach to NMR structure determination. *Journal of Biomolecular NMR*, **1998**, 11, 241-63	3	16
58	Relativistic effects on molecular hyperfine interactions: Application to ytterbium fluorides. *Journal of Chemical Physics*, **1984**, 80, 3270-3277	3.9	16

57	Nuclear magnetic resonance studies of ligand-exchange processes. II. Kinetics of configurational rearrangement for some mixed .beta.-diketonate complexes of gallium(III). *Inorganic Chemistry*, **1969**, 8, 644-648	5.1	16
56	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
55	Cryptic binding sites become accessible through surface reconstruction of the type I collagen fibril. *Scientific Reports*, **2018**, 8, 16646	4.9	16
54	Rapid and accurate determination of atomistic RNA dynamic ensemble models using NMR and structure prediction. *Nature Communications*, **2020**, 11, 5531	17.4	15
53	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and Schr□dinger FEP. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 533-9	4.2	15
52	Low-Resolution Molecular Dynamics Simulations of the 30S Ribosomal Subunit. *Multiscale Modeling and Simulation*, **2006**, 5, 1248-1263	1.8	14
51	Stable and efficient algorithms for X□multiple scattering calculations. *International Journal of Quantum Chemistry*, **1980**, 18, 1091-1099	2.1	14
50	Extracting water and ion distributions from solution x-ray scattering experiments. *Journal of Chemical Physics*, **2016**, 144, 214105	3.9	14
49	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
48	An Empirical Analysis of Proton Chemical Shifts in Nucleic Acids. *ACS Symposium Series*, **1999**, 194-206	0.4	13
47	Dynamical simulation of rate constants in protein-ligand interactions. *Progress in Biophysics and Molecular Biology*, **1988**, 52, 39-70	4.7	13
46	The bonding of CO to a platinum surface: relativistic cluster studies. *Chemical Physics Letters*, **1981**, 81, 170-174	2.5	13
45	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
44	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
43	Diffuse X-ray scattering from correlated motions in a protein crystal. *Nature Communications*, **2020**, 11, 1271	17.4	12
42	Chapter 4:Integral Equation Theory of Biomolecules and Electrolytes. *RSC Biomolecular Sciences*, **2012**, 51-86		12
41	A novel method for finding tRNA genes. *Rna*, **2003**, 9, 507-17	5.8	12
40	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

39	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
38	Electronic structures of active site models for compounds I and II of peroxidase. *Journal of the American Chemical Society*, **1985**, 107, 4013-4015	16.4	11
37	Interpretation of CO/Pt photoemission data via relattvistic cluster calculations. *Surface Science*, **1981**, 106, 523-528	1.8	11
36	Solution NMR readily reveals distinct structural folds and interactions in doubly C- and F-labeled RNAs. *Science Advances*, **2020**, 6,	14.3	11
35	X.alpha. multiple-scattering study of hexacyanoferrate(III). *Inorganic Chemistry*, **1981**, 20, 528-533	5.1	10
34	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
33	Electronic structure of octachloroditungstate(II). *Inorganic Chemistry*, **1984**, 23, 3271-3273	5.1	9
32	Molecular Dynamics Simulations of Macromolecular Crystals. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1402	7.9	9
31	Propagated Perturbations from a Peripheral Mutation Show Interactions Supporting WW Domain Thermostability. *Structure*, **2018**, 26, 1474-1485.e5	5.2	9
30	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
29	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
28	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
27	Deleterious effects of carbon-carbon dipolar coupling on RNA NMR dynamics. *Journal of Biomolecular NMR*, **2020**, 74, 321-331	3	7
26	The Ornstein–Zernike equation in molecular electronic structure theory. *Molecular Physics*, **2010**, 108, 307-314	1.7	7
25	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
24	The Interplay between Molten Globules and Heme Disassociation Defines Human Hemoglobin Disassembly. *Biophysical Journal*, **2020**, 118, 1381-1400	2.9	6
23	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
22	Vectorization of the generalized Born model for molecular dynamics on shared-memory computers. *Computational and Theoretical Chemistry*, **2001**, 549, 193-201		6

21	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
20	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
19	Theory and applications of the generalized born solvation model in macromolecular simulations **2000**, 56, 275		5
18	Relativistic molecular orbital theory of zero-field splittings in triplets. *Chemical Physics Letters*, **1984** , 109, 66-70	2.5	4
17	Insulator□onductor transition in tetracyanoplatinate complexes. *Chemical Physics Letters*, **1982**, 91, 353-357	2.5	4
16	Using quantum chemistry to estimate chemical shifts in biomolecules. *Biophysical Chemistry*, **2020**, 267, 106476	3.5	4
15	Links between the charge model and bonded parameter force constants in biomolecular force fields. *Journal of Chemical Physics*, **2017**, 147, 161730	3.9	3
14	High-resolution solution structure of Bacillus subtilis IIAglc **1998**, 31, 258-270		3
13	Atomistic Simulations of Heme Dissociation Pathways in Human Methemoglobins Reveal Hidden Intermediates. *Biochemistry*, **2020**, 59, 4093-4107	3.2	3
12	Coupled intra- and interdomain dynamics support domain cross-talk in Pin1. *Journal of Biological Chemistry*, **2020**, 295, 16585-16603	5.4	2
11	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
10	NMR Parameters in Proteins and Nucleic Acids **2004**, 339-351		1
9	Integral equation models for solvent in macromolecular crystals.. *Journal of Chemical Physics*, **2022**, 156, 014801	3.9	1
8	Simulations of Kindlin-2 PIP binding domains reveal protonation-dependent membrane binding modes. *Biophysical Journal*, **2021**,	2.9	1
7	Drug-Target Binding Forces: Advances in Force Field Approaches **2003**, 169-185		1
6	A quantitative model predicts how m6A reshapes the kinetic landscape of nucleic acid hybridization and conformational transitions		1
5	Refinement of RNA Structures Using Amber Force Fields. *Crystals*, **2021**, 11,	2.3	1
4	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	

3 Implicit Solvent Models and Electrostatics in Molecular Recognition **2012**, 171-189

2 In Silico: An Alternate Approach to Chemistry and Biology **2011**, 19-31

1 Perspective on Dynamics of folded proteins *Theoretical Chemistry Accounts*, **2000**, 103, 332-334 1.9