David A Case

List of Publications by Year
in descending order

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253 papers	78,692 citations	3151 92 h-index	735 251 g-index
272 all docs	272 docs citations	272 times ranked	50140 citing authors

#	Article	IF	Citations
1	Development and testing of a general amber force field. Journal of Computational Chemistry, 2004, 25, 1157-1174.	1.5	14,342
2	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	1.5	7,742
3	A new force field for molecular mechanical simulation of nucleic acids and proteins. Journal of the American Chemical Society, 1984, 106, 765-784.	6.6	4,802
4	Automatic atom type and bond type perception in molecular mechanical calculations. Journal of Molecular Graphics and Modelling, 2006, 25, 247-260.	1.3	4,173
5	Calculating Structures and Free Energies of Complex Molecules:â€‰ Combining Molecular Mechanics and Continuum Models. Accounts of Chemical Research, 2000, 33, 889-897.	7.6	4,098
6	An all atom force field for simulations of proteins and nucleic acids. Journal of Computational Chemistry, 1986, 7, 230-252.	1.5	3,292
7	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.	3.0	2,839
8	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, 405-413.	2.3	2,567
9	Exploring protein native states and large-scale conformational changes with a modified generalized born model. Proteins: Structure, Function and Bioinformatics, 2004, 55, 383-394.	1.5	2,068
10	An overview of the Amber biomolecular simulation package. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 198-210.	6.2	1,734
11	Force Fields for Protein Simulations. Advances in Protein Chemistry, 2003, 66, 27-85.	4.4	1,560
12	Continuum Solvent Studies of the Stability of DNA, RNA, and Phosphoramidateâ’DNA Helices. Journal of the American Chemical Society, 1998, 120, 9401-9409.	6.6	1,442
13	Insights into Proteinâ€“Protein Binding by Binding Free Energy Calculation and Free Energy Decomposition for the Rasâ€“Raf and Rasâ€“RalGDS Complexes. Journal of Molecular Biology, 2003, 330, 891-913.	2.0	1,079
14	GENERALIZEDBORNMODELS OFMACROMOLECULARSOLVATIONEFFECTS. Annual Review of Physical Chemistry, 2000, 51, 129-152.	4.8	1,073
15	Modification of the Generalized Born Model Suitable for Macromolecules. Journal of Physical Chemistry B, 2000, 104, 3712-3720.	1.2	973
16	Theory and applications of the generalized born solvation model in macromolecular simulations. Biopolymers, 2000, 56, 275-291.	1.2	878
17	Parmbsc1: a refined force field for DNA simulations. Nature Methods, 2016, 13, 55-58.	9.0	790
18	Converging free energy estimates: MM-PB(GB)SA studies on the protein-protein complex Ras-Raf. Journal of Computational Chemistry, 2004, 25, 238-250.	1.5	750

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19	DOCK 6: Combining techniques to model RNAâ€“small molecule complexes. Rna, 2009, 15, 1219-1230.	1.6	616
20	Structural basis for DNA bending by the architectural transcription factor LEF-1. Nature, 1995, 376, 791-795.	13.7	582
21	Density-Functional Theory of Spin Polarization and Spin Coupling in Ironâ€”Sulfur Clusters. Advances in Inorganic Chemistry, 1992, 38, 423-470.	0.4	570
22	DOCK 6: Impact of new features and current docking performance. Journal of Computational Chemistry, 2015, 36, 1132-1156.	1.5	552
23	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. Journal of Computational Chemistry, 2004, 25, 265-284.	1.5	523
24	Constant pH molecular dynamics in generalized Born implicit solvent. Journal of Computational Chemistry, 2004, 25, 2038-2048.	1.5	450
25	RNAMotif, an RNA secondary structure definition and search algorithm. Nucleic Acids Research, 2001, 29, 4724-4735.	6.5	421
26	Effective Born radii in the generalized Born approximation: The importance of being perfect. Journal of Computational Chemistry, 2002, 23, 1297-1304.	1.5	412
27	Molecular Dynamics Simulations of Nucleic Acids with a Generalized Born Solvation Model. Journal of the American Chemical Society, 2000, 122, 2489-2498.	6.6	398
28	The implementation of a fast and accurate QM/MM potential method in Amber. Journal of Computational Chemistry, 2008, 29, 1019-1031.	1.5	360
29	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.	6.5	349
30	Generalized Born Model with a Simple, Robust Molecular Volume Correction. Journal of Chemical Theory and Computation, 2007, 3, 156-169.	2.3	334
31	Density Functional/Poisson-Boltzmann Calculations of Redox Potentials for Iron-Sulfur Clusters. Journal of the American Chemical Society, 1994, 116, 11898-11914.	6.6	305
32	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.	2.5	293
33	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.	6.6	288
34	A new analysis of proton chemical shifts in proteins. Journal of the American Chemical Society, 1991, 113, 9436-9444.	6.6	288
35	Application of a pairwise generalized Born model to proteins and nucleic acids: inclusion of salt effects. Theoretical Chemistry Accounts, 1999, 101, 426-434.	0.5	282
36	High-resolution solution structures of oxidized and reduced Escherichia coli thioredoxin. Structure, 1994, 2, 853-868.	1.6	281

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37	Nonlinear scaling schemes for Lennard-Jones interactions in free energy calculations. Journal of Chemical Physics, 2007, 127, 214108.	1.2	269
38	Proton Binding to Proteins:Â pKaCalculations with Explicit and Implicit Solvent Models. Journal of the American Chemical Society, 2004, 126, 4167-4180.	6.6	266
39	Automated prediction of 15N, 13Calpha, 13Cbeta and 13C' chemical shifts in proteins using a density functional database. Journal of Biomolecular NMR, 2001, 21, 321-333.	1.6	262
40	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, 3799-3813.	0.2	245
41	Three-Dimensional Molecular Theory of Solvation Coupled with Molecular Dynamics in Amber. Journal of Chemical Theory and Computation, 2010, 6, 607-624.	2.3	232
42	Broken symmetry analysis of spin coupling in iron-sulfur clusters. Journal of the American Chemical Society, 1988, 110, 1001-1005.	6.6	225
43	Simulations of peptide conformational dynamics and thermodynamics. Chemical Reviews, 1993, 93, 2487-2502.	23.0	224
44	Density Functional and Reduction Potential Calculations of Fe4S4Clusters. Journal of the American Chemical Society, 2003, 125, 1923-1936.	6.6	220
45	Electronic structure of Ru2(O2CR)4+ and Rh2(O2CR)4+ complexes. Journal of the American Chemical Society, 1979, 101, 5256-5267.	6.6	217
46	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, 3721-3740.	0.2	216
47	Implementation of the SCC-DFTB Method for Hybrid QM/MM Simulations within the Amber Molecular Dynamics Packageâ€. Journal of Physical Chemistry A, 2007, 111, 5655-5664.	1.1	213
48	Structure of the HIV-1 RNA packaging signal. Science, 2015, 348, 917-921.	6.0	211
49	Continuum Solvent Studies of the Stability of RNA Hairpin Loops and Helices. Journal of Biomolecular Structure and Dynamics, 1998, 16, 671-682.	2.0	210
50	Optimized particle-mesh Ewald/multiple-time step integration for molecular dynamics simulations. Journal of Chemical Physics, 2001, 115, 4003-4018.	1.2	194
51	Characterization of Domainâ€“Peptide Interaction Interface: A Case Study on the Amphiphysin-1 SH3 Domain. Journal of Molecular Biology, 2008, 376, 1201-1214.	2.0	194
52	Molecular Dynamics and NMR Spin Relaxation in Proteins. Accounts of Chemical Research, 2002, 35, 325-331.	7.6	193
53	An accurate and simple quantum model for liquid water. Journal of Chemical Physics, 2006, 125, 184507.	1.2	187
54	Lessons learned from comparing molecular dynamics engines on the SAMPL5 dataset. Journal of Computer-Aided Molecular Design, 2017, 31, 147-161.	1.3	187

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55	Î¼ABC: a systematic microsecond molecular dynamics study of tetranucleotide sequence effects in B-DNA. Nucleic Acids Research, 2014, 42, 12272-12283.	6.5	186
56	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, 265-280.	2.0	183
57	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.	2.0	182
58	FeMo Cofactor of Nitrogenase:Â A Density Functional Study of States MN, MOX, MR, and MI. Journal of the American Chemical Society, 2001, 123, 12392-12410.	6.6	181
59	The structure of calcyclin reveals a novel homodimeric fold for S100 Ca2+-binding proteins. Nature Structural and Molecular Biology, 1995, 2, 790-796.	3.6	180
60	Softâ€core potentials in thermodynamic integration: Comparing oneâ€•and twoâ€step transformations. Journal of Computational Chemistry, 2011, 32, 3253-3263.	1.5	178
61	Dynamics of ligand escape from the heme pocket of myoglobin. Journal of the American Chemical Society, 1988, 110, 7690-7697.	6.6	172
62	Incorporating Solvation Effects into Density Functional Electronic Structure Calculations. The Journal of Physical Chemistry, 1994, 98, 11059-11068.	2.9	171
63	Rescoring Docking Hit Lists for Model Cavity Sites: Predictions and Experimental Testing. Journal of Molecular Biology, 2008, 377, 914-934.	2.0	168
64	Theories of chemical shift anisotropies in proteins and nucleic acids. Progress in Nuclear Magnetic Resonance Spectroscopy, 1998, 32, 165-190.	3.9	164
65	Estimation of Absolute Free Energies of Hydration Using Continuum Methods:â€‰ Accuracy of Partial Charge Models and Optimization of Nonpolar Contributions. Journal of Chemical Theory and Computation, 2006, 2, 128-139.	2.3	163
66	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, 3926-3947.	2.3	161
67	Twentyâ€five years of nucleic acid simulations. Biopolymers, 2013, 99, 969-977.	1.2	157
68	Generalized Born Implicit Solvent Models for Biomolecules. Annual Review of Biophysics, 2019, 48, 275-296.	4.5	155
69	Structural, Spectroscopic, and Redox Consequences of a Central Ligand in the FeMoco of Nitrogenase:â€‰ A Density Functional Theoretical Study. Journal of the American Chemical Society, 2003, 125, 8377-8383.	6.6	146
70	Biomolecular simulations at constant pH. Current Opinion in Structural Biology, 2005, 15, 157-163.	2.6	144
71	Unfolding of an ?-helix in water. Biopolymers, 1991, 31, 1351-1361.	1.2	140
72	Insights into the Mobility of Methyl-Bearing Side Chains in Proteins from3JCCand3JCNCouplings. Journal of the American Chemical Society, 2003, 125, 8959-8966.	6.6	131

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73	Evaluating Rotational Diffusion from Protein MD Simulations. Journal of Physical Chemistry B, 2008, 112, 6013-6024.	1.2	131
74	Molecular dynamics analysis of NMR relaxation in a zinc-finger peptide. Journal of the American Chemical Society, 1992, 114, 9059-9067.	6.6	118
75	Density functional calculation of pK a values and redox potentials in the bovine Rieske iron-sulfur protein. Journal of Biological Inorganic Chemistry, 2002, 7, 632-639.	1.1	117
76	Domain packing and dynamics in the DNA complex of the N-terminal zinc fingers of TFIIIA. Nature Structural Biology, 1997, 4, 605-608.	9.7	116
77	High-resolution solution structure of reduced French bean plastocyanin and comparison with the crystal structure of poplar plastocyanin. Journal of Molecular Biology, 1991, 221, 533-555.	2.0	114
78	Including Side Chain Flexibility in Continuum Electrostatic Calculations of Protein Titration. The Journal of Physical Chemistry, 1996, 100, 20156-20163.	2.9	113
79	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, 317-331.	1.6	112
80	[13] Use of chemical shifts and coupling constants in nuclear magnetic resonance structural studies on peptides and proteins. Methods in Enzymology, 1994, 239, 392-416.	0.4	111
81	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.	6.6	110
82	NGLviewâ€“interactive molecular graphics for Jupyter notebooks. Bioinformatics, 2018, 34, 1241-1242.	1.8	110
83	Calculations of NMR dipolar coupling strengths in model peptides. Journal of Biomolecular NMR, 1999, 15, 95-102.	1.6	109
84	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, 322-337.	1.5	106
85	NMR Solution Structure of Cu(I) Rusticyanin fromThiobacillus ferrooxidans: Structural Basis for the Extreme Acid Stability and Redox Potential. Journal of Molecular Biology, 1996, 263, 752-767.	2.0	104
86	Solution Structure of Carbonmonoxy Myoglobin Determined from Nuclear Magnetic Resonance Distance and Chemical Shift Constraints. Journal of Molecular Biology, 1994, 244, 183-197.	2.0	103
87	Ion Counting from Explicit-Solvent Simulations and 3D-RISM. Biophysical Journal, 2014, 106, 883-894.	0.2	102
88	The calculation of one-electron properties from XÎ± multiple scattering wavefunctions. Chemical Physics Letters, 1976, 39, 33-38.	1.2	98
89	Static and Dynamic Effects on Vicinal ScalarJCouplings in Proteins and Peptides:Â A MD/DFT Analysis. Journal of the American Chemical Society, 2000, 122, 10390-10397.	6.6	97
90	Characterization of the Fe Site in Ironâ^'Sulfur Cluster-Free Hydrogenase (Hmd) and of a Model Compound via Nuclear Resonance Vibrational Spectroscopy (NRVS). Inorganic Chemistry, 2008, 47, 3969-3977.	1.9	97

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91	Evaluating Î²-turn mimics as Î²-sheet folding nucleators. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11067-11072.	3.3	97
92	Characterization of Domain-Peptide Interaction Interface. Molecular and Cellular Proteomics, 2009, 8, 639-649.	2.5	96
93	Derivation of Fixed Partial Charges for Amino Acids Accommodating a Specific Water Model and Implicit Polarization. Journal of Physical Chemistry B, 2013, 117, 2328-2338.	1.2	95
94	X.alpha. multiple scattering calculations on copper porphine. Journal of the American Chemical Society, 1977, 99, 6182-6194.	6.6	93
95	RNAML: A standard syntax for exchanging RNA information. Rna, 2002, 8, 707-717.	1.6	91
96	Density Functional Study on the Electronic Structures of Model Peroxidase Compounds I and II. Journal of the American Chemical Society, 1997, 119, 11442-11451.	6.6	90
97	Testing if the Interstitial Atom, X, of the Nitrogenase Molybdenumâ^'Iron Cofactor Is N or C:â€‰ ENDOR, ESEEM, and DFT Studies of the S = ³/₂ Resting State in Multiple Environments. Inorganic Chemistry, 2007, 46, 11437-11449.	1.9	89
98	ff14ipq: A Self-Consistent Force Field for Condensed-Phase Simulations of Proteins. Journal of Chemical Theory and Computation, 2014, 10, 4515-4534.	2.3	87
99	Density Functional Calculations of Proton Chemical Shifts in Model Peptides. Journal of the American Chemical Society, 1997, 119, 12262-12273.	6.6	85
100	Extended Sugar-Assisted Glycopeptide Ligations:â€‰ Development, Scope, and Applications. Journal of the American Chemical Society, 2007, 129, 13527-13536.	6.6	84
101	A Multistep Approach to Structure-Based Drug Design:â€‰ Studying Ligand Binding at the Human Neutrophil Elastase. Journal of Medicinal Chemistry, 2006, 49, 1837-1844.	2.9	78
102	Major groove width variations in RNA structures determined by NMR and impact of 13C residual chemical shift anisotropy and 1Hâ€“13C residual dipolar coupling on refinement. Journal of Biomolecular NMR, 2010, 47, 205-219.	1.6	77
103	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, 12811-12824.	1.2	77
104	Advanced Potential Energy Surfaces for Molecular Simulation. Journal of Physical Chemistry B, 2016, 120, 9811-9832.	1.2	77
105	Characterization of biomolecular structure and dynamics by NMR cross relaxation. Progress in Nuclear Magnetic Resonance Spectroscopy, 1994, 26, 27-58.	3.9	76
106	A Phototautomerizable Model DNA Base Pair. Journal of the American Chemical Society, 2000, 122, 9917-9920.	6.6	76
107	Structural basis for transcriptional start site control of HIV-1 RNA fate. Science, 2020, 368, 413-417.	6.0	76
108	NMR solution structure of the inserted domain of human leukocyte function associated antigen-1. Journal of Molecular Biology, 2000, 295, 1251-1264.	2.0	74

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109	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.	1.2	74
110	Symmetry and Bonding in Metalloporphyrins. A Modern Implementation for the Bonding Analyses of Five- and Six-Coordinate High-Spin Iron(III)â˜Porphyrin Complexes through Density Functional Calculation and NMR Spectroscopy. Journal of the American Chemical Society, 2003, 125, 6774-6783.	6.6	74
111	How Nitrogenase Shakes â˜ Initial Information about Pâ˜Cluster and FeMo-cofactor Normal Modes from Nuclear Resonance Vibrational Spectroscopy (NRVS). Journal of the American Chemical Society, 2006, 128, 7608-7612.	6.6	73
112	Quantum dynamical effects in liquid water: A semiclassical study on the diffusion and the infrared absorption spectrum. Journal of Chemical Physics, 2009, 131, 164509.	1.2	73
113	Computational methods for determining protein structures from NMR data. Biochemical Pharmacology, 1990, 40, 15-22.	2.0	72
114	Induced Fit and â€œLock and Keyâ€•Recognition of 5S RNA by Zinc Fingers of Transcription Factor IIIA. Journal of Molecular Biology, 2006, 357, 275-291.	2.0	72
115	Nature of the iron-oxygen bond in oxyhemoglobin. Journal of the American Chemical Society, 1977, 99, 6103-6105.	6.6	66
116	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, 825-836.	1.5	66
117	Relativistic scattered wave calculations on UF6. Journal of Chemical Physics, 1980, 72, 3443-3448.	1.2	65
118	Density Functional Study of Ribose and Deoxyribose Chemical Shifts. Journal of Physical Chemistry A, 1998, 102, 5280-5289.	1.1	63
119	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, 15002-15021.	6.6	63
120	Simple electrolyte solutions: Comparison of DRISM and molecular dynamics results for alkali halide solutions. Journal of Chemical Physics, 2013, 138, 044103.	1.2	63
121	Application ofXÎ± multipleâ€scattering theory to planar organic molecules: Oneâ€electron properties and ionization potentials of benzene, pyridine, pyrazine, pyrrole, and imidazole. Journal of Chemical Physics, 1980, 73, 3294-3313.	1.2	62
122	DNA oligonucleotides with A, T, G or C opposite an abasic site: structure and dynamics. Nucleic Acids Research, 2008, 36, 253-262.	6.5	60
123	High-Resolution ENDOR Spectroscopy Combined with Quantum Chemical Calculations Reveals the Structure of Nitrogenase Janus Intermediate E₄(4H). Journal of the American Chemical Society, 2019, 141, 11984-11996.	6.6	58
124	Dynamics of a type VI reverse turn in a linear peptide in aqueous solution. Folding & Design, 1997, 2, 35-46.	4.5	57
125	NMR and molecular dynamics studies of the hydration of a zinc finger-DNA complex 1 1Edited by M. F. Summers. Journal of Molecular Biology, 2000, 302, 1101-1117.	2.0	57
126	Ligand-Bound S = ¹/₂ FeMo-Cofactor of Nitrogenase: Hyperfine Interaction Analysis and Implication for the Central Ligand X Identity. Inorganic Chemistry, 2008, 47, 6162-6172.	1.9	57

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127	Relativistic effects on molecular hyperfine interactions: Application to XeF and CsO. Journal of Chemical Physics, 1983, 79, 4939-4949.	1.2	56
128	A new model for chemical shifts of amide hydrogens in proteins. Journal of Biomolecular NMR, 2007, 38, 139-150.	1.6	56
129	AFNMR: automated fragmentation quantum mechanical calculation of NMR chemical shifts for biomolecules. Journal of Biomolecular NMR, 2015, 63, 125-139.	1.6	56
130	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, 15612-15617.	6.6	55
131	Metal Substitution in the Active Site of Nitrogenase MFe7S9(M = Mo4+, V3+, Fe3+). Inorganic Chemistry, 2002, 41, 5744-5753.	1.9	53
132	Direct Simulation of Electron Transfer Reactions in DNA Radical Cations. Journal of Physical Chemistry B, 2008, 112, 16935-16944.	1.2	53
133	Carbonâ˜'Deuterium Bonds as Probes of Dihydrofolate Reductase. Journal of the American Chemical Society, 2008, 130, 6597-6603.	6.6	53
134	Structural Details, Pathways, and Energetics of Unfolding Apomyoglobin. Journal of Molecular Biology, 2003, 325, 555-567.	2.0	52
135	Molecular dynamics simulation of triclinic lysozyme in a crystal lattice. Protein Science, 2016, 25, 87-102.	3.1	52
136	Structure of the 30ÂkDa HIV-1 RNA Dimerization Signal by a Hybrid Cryo-EM, NMR, and Molecular Dynamics Approach. Structure, 2018, 26, 490-498.e3.	1.6	52
137	Rapid and accurate determination of atomistic RNA dynamic ensemble models using NMR and structure prediction. Nature Communications, 2020, 11, 5531.	5.8	52
138	[9] Calculations of proton-binding thermodynamics in proteins. Methods in Enzymology, 1998, 295, 170-189.	0.4	51
139	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.	1.3	50
140	Collective NMR relaxation model applied to protein dynamics. Physical Review Letters, 1994, 72, 940-943.	2.9	49
141	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.	6.6	48
142	High resolution solution structure of a DNA duplex alkylated by the antitumor agent duocarmycin SA. Journal of Molecular Biology, 1997, 272, 237-252.	2.0	47
143	FeMo cofactor of nitrogenase: energetics and local interactions in the protein environment. Journal of Biological Inorganic Chemistry, 2002, 7, 735-749.	1.1	47
144	Nudged Elastic Band Calculation of Minimal Energy Paths for the Conformational Change of a GG Non-canonical Pair. Journal of Molecular Biology, 2006, 357, 1683-1693.	2.0	47

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145	Peptide Crystal Simulations Reveal Hidden Dynamics. Journal of the American Chemical Society, 2013, 135, 7938-7948.	6.6	47
146	Competitive interaction of monovalent cations with DNA from 3D-RISM. Nucleic Acids Research, 2015, 43, 8405-8415.	6.5	47
147	XÎ± multiple scattering calculations on iron(II) porphine. Journal of Chemical Physics, 1983, 79, 2881-2892.	1.2	46
148	Binding Modes for the First Coupled Electron and Proton Addition to FeMoco of Nitrogenase. Journal of the American Chemical Society, 2002, 124, 4546-4547.	6.6	46
149	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, 11016-11021.	3.3	46
150	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.	6.6	46
151	Water-induced polaron formation at the pentacene surface: Quantum mechanical molecular mechanics simulations. Physical Review B, 2009, 79, .	1.1	44
152	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.	2.3	44
153	The Dependence of Carbohydrateâ€“Aromatic Interaction Strengths on the Structure of the Carbohydrate. Journal of the American Chemical Society, 2016, 138, 7636-7648.	6.6	44
154	Assessment of zinc finger orientations by residual dipolar coupling constants. Journal of Biomolecular NMR, 2000, 16, 9-21.	1.6	43
155	Flexibility of an Antibody Binding Site Measured with Photon Echo Spectroscopy. Journal of Physical Chemistry B, 2002, 106, 1090-1103.	1.2	43
156	Chemical shifts in biomolecules. Current Opinion in Structural Biology, 2013, 23, 172-176.	2.6	43
157	Calculation of chemical shift anisotropy in proteins. Journal of Biomolecular NMR, 2011, 51, 303-312.	1.6	41
158	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, 2530-2543.	6.6	41
159	Stereochemistry of carbon monoxide binding to myoglobin and hemoglobin. Journal of Molecular Biology, 1978, 123, 697-701.	2.0	40
160	NMR Structure of a Cyclic Polyamideâ^'DNA Complex. Journal of the American Chemical Society, 2004, 126, 7958-7966.	6.6	40
161	NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Nature Structural and Molecular Biology, 2015, 22, 433-434.	3.6	40
162	Spinâ€orbit and spinâ€polarization effects in neptunium hexafluoride. Journal of Chemical Physics, 1985, 83, 5792-5796.	1.2	39

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163	Thermodynamics of a reverse turn motif. Solvent effects and side-chain packing. Journal of Molecular Biology, 1997, 270, 305-317.	2.0	39
164	Evaluation of DNA Force Fields in Implicit Solvation. Journal of Chemical Theory and Computation, 2011, 7, 3181-3198.	2.3	38
165	Diffuse X-ray scattering from correlated motions in a protein crystal. Nature Communications, 2020, 11, 1271.	5.8	37
166	Density-functional calculations of spin coupling in [Fe4S4]3+ clusters. International Journal of Quantum Chemistry, 1995, 56, 95-102.	1.0	36
167	Modeling of Flap Endonuclease Interactions with DNA Substrate. Journal of Molecular Biology, 2003, 328, 537-554.	2.0	36
168	Reintroducing electrostatics into protein X-ray structure refinement: bulk solvent treated as a dielectric continuum. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 2094-2103.	2.5	32
169	Vibrational averaging of chemical shift anisotropies in model peptides. Journal of Biomolecular NMR, 2007, 38, 255-266.	1.6	31
170	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, 12954-12965.	6.6	31
171	Solution structure and dynamics of yeast elongin C in complex with a von hippel-lindau peptide 1 1Edited by M. F. Summers. Journal of Molecular Biology, 2001, 312, 177-186.	2.0	30
172	Multiscale modeling of nucleic acids: Insights into DNA flexibility. Biopolymers, 2008, 89, 722-731.	1.2	30
173	Atomic structures of excited state Aâ€“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.	1.6	30
174	Molecular dynamics analysis of a flexible loop at the binding interface of the <scp>SARSâ€CoV</scp>â€2 spike protein <scp>receptorâ€binding</scp> domain. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1044-1053.	1.5	30
175	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.	6.6	29
176	Feâ€“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, 409-420.	1.6	29
177	Energetic Selection of Topology in Ferredoxins. PLoS Computational Biology, 2012, 8, e1002463.	1.5	29
178	Solution NMR readily reveals distinct structural folds and interactions in doubly ¹³ C- and ¹⁹ F-labeled RNAs. Science Advances, 2020, 6, .	4.7	29
179	Improved chemistry restraints for crystallographic refinement by integrating the Amber force field into Phenix. Acta Crystallographica Section D: Structural Biology, 2020, 76, 51-62.	1.1	29
180	The structural basis for in situ activation of DNA alkylation by duocarmycin SA11Edited by I. Tinoco. Journal of Molecular Biology, 2000, 300, 1195-1204.	2.0	28

#	Article	IF	Citations
181	Sucrose in aqueous solution revisited, Part 1: Molecular dynamics simulations and direct and indirect dipolar coupling analysis. Biopolymers, 2012, 97, 276-288.	1.2	28
182	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	1.2	28
183	Dynamic Simulations of Oxygen Binding to Myoglobin. Annals of the New York Academy of Sciences, 1986, 482, 222-233.	1.8	27
184	Second derivatives in generalized Born theory. Journal of Computational Chemistry, 2006, 27, 1662-1675.	1.5	27
185	Structural fidelity and NMR relaxation analysis in a prototype RNA hairpin. Rna, 2015, 21, 963-974.	1.6	27
186	Large Variations in One-Bond 13CÎ±â^'13CÎ² J Couplings in Polypeptides Correlate with Backbone Conformation. Journal of the American Chemical Society, 2000, 122, 2168-2171.	6.6	26
187	Multi-Level Ewald: A Hybrid Multigrid/Fast Fourier Transform Approach to the Electrostatic Particle-Mesh Problem. Journal of Chemical Theory and Computation, 2010, 6, 443-458.	2.3	26
188	Dynamic Water-Mediated Hydrogen Bonding in a Collagen Model Peptide. Biochemistry, 2015, 54, 6029-6037.	1.2	26
189	Continuum solvent molecular dynamics study of flexibility in interleukin-8. Journal of Molecular Graphics and Modelling, 2001, 19, 136-145.	1.3	25
190	The importance of protonation and tautomerization in relative binding affinity prediction: a comparison of AMBER TI and SchrÃ¶dinger FEP. Journal of Computer-Aided Molecular Design, 2016, 30, 533-539.	1.3	25
191	Molecular dynamics simulations of macromolecular crystals. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1402.	6.2	25
192	Molecular Dynamics Docking Driven by NMR-Derived Restraints to Determine the Structure of the Calicheamicin Î³1I Oligosaccharide Domain Complexed to Duplex DNA. Magnetic Resonance in Chemistry, 1996, 34, S147-S155.	1.1	24
193	Molecular dynamics analysis of a ribonuclease C-peptide analogue. Biopolymers, 1993, 33, 1567-1580.	1.2	23
194	Comparison of SARS and NL63 Papain-Like Protease Binding Sites and Binding Site Dynamics: Inhibitor Design Implications. Journal of Molecular Biology, 2011, 414, 272-288.	2.0	23
195	Cryptic binding sites become accessible through surface reconstruction of the type I collagen fibril. Scientific Reports, 2018, 8, 16646.	1.6	23
196	Predicting interactions of winged-helix transcription factors with DNA. Proteins: Structure, Function and Bioinformatics, 2004, 57, 172-187.	1.5	22
197	Resolving Ambiguous Protonation and Oxidation States in the Oxygen Evolving Complex of Photosystem II. Journal of Physical Chemistry B, 2018, 122, 8654-8664.	1.2	22
198	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.	1.1	22

#	Article	IF	Citations
199	The circumsphere as a tool to assess distortion in [4Fe-4S] atom clusters. Journal of Biological Inorganic Chemistry, 2003, 8, 519-526.	1.1	21
200	Revealing Accessibility of Cryptic Protein Binding Sites within the Functional Collagen Fibril. Biomolecules, 2017, 7, 76.	1.8	21
201	Distributed torsion angle grid search in high dimensions: a systematic approach to NMR structure determination. Journal of Biomolecular NMR, 1998, 11, 241-263.	1.6	20
202	All-atom crystal simulations of DNA and RNA duplexes. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1059-1071.	1.1	20
203	Systematic Comparison of Amber and Rosetta Energy Functions for Protein Structure Evaluation. Journal of Chemical Theory and Computation, 2018, 14, 6015-6025.	2.3	20
204	Kinetics of stereochemical rearrangements for mixed .beta.-diketonate complexes of aluminum(III). Inorganic Chemistry, 1971, 10, 482-486.	1.9	19
205	A Combined 2D-NMR and Molecular Dynamics Analysis of the Structure of the Actinomycin D: d(ATGCAT)2Complex. Journal of Biomolecular Structure and Dynamics, 1989, 6, 929-969.	2.0	19
206	Relativistic scattered wave calculations of hexachloroâ€•and hexabromoiridate (IV). Journal of Chemical Physics, 1984, 81, 4554-4563.	1.2	18
207	Searching and Optimizing Structure Ensembles for Complex Flexible Sugars. Journal of the American Chemical Society, 2011, 133, 15252-15255.	6.6	18
208	A quantitative model predicts how m6A reshapes the kinetic landscape of nucleic acid hybridization and conformational transitions. Nature Communications, 2021, 12, 5201.	5.8	18
209	An Empirical Analysis of Proton Chemical Shifts in Nucleic Acids. ACS Symposium Series, 1999, , 194-206.	0.5	17
210	Characterizing Watsonâ€“Crick versus Hoogsteen Base Pairing in a DNAâ€“Protein Complex Using Nuclear Magnetic Resonance and Site-Specifically 13C- and 15N-Labeled DNA. Biochemistry, 2019, 58, 1963-1974.	1.2	17
211	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.	1.9	16
212	Relativistic effects on molecular hyperfine interactions: Application to ytterbium fluorides. Journal of Chemical Physics, 1984, 80, 3270-3277.	1.2	16
213	A novel method for finding tRNA genes. Rna, 2003, 9, 507-517.	1.6	16
214	A twist in the road less traveled: The AMBER ff15ipq-m force field for protein mimetics. Journal of Chemical Physics, 2020, 153, .	1.2	16
215	Lowâ€Resolution Molecular Dynamics Simulations of the 30S Ribosomal Subunit. Multiscale Modeling and Simulation, 2006, 5, 1248-1263.	0.6	15
216	Integral Equation Theory of Biomolecules and Electrolytes. RSC Biomolecular Sciences, 2012, , 51-86.	0.4	15

#	Article	IF	Citations
217	Extracting water and ion distributions from solution x-ray scattering experiments. Journal of Chemical Physics, 2016, 144, 214105.	1.2	15
218	Stable and efficient algorithms for X Î± multiple scattering calculations. International Journal of Quantum Chemistry, 1980, 18, 1091-1099.	1.0	14
219	Dynamical simulation of rate constants in protein-ligand interactions. Progress in Biophysics and Molecular Biology, 1988, 52, 39-70.	1.4	14
220	Design and synthesis of highly constrained factor Xa inhibitors: amidine-Substituted bis(benzoyl)-[and]-diazepan-2-ones and bis(benzylidene)-bis(gem-dimethyl)cycloketones. Bioorganic and Medicinal Chemistry, 2003, 11, 3379-3392.	1.4	14
221	Sucrose in aqueous solution revisited, Part 2: Adaptively biased molecular dynamics simulations and computational analysis of NMR relaxation. Biopolymers, 2012, 97, 289-302.	1.2	14
222	Propagated Perturbations from a Peripheral Mutation Show Interactions Supporting WW Domain Thermostability. Structure, 2018, 26, 1474-1485.e5.	1.6	14
223	The bonding of CO to a platinum surface: relativistic cluster studies. Chemical Physics Letters, 1981, 81, 170-174.	1.2	13
224	The Interplay between Molten Globules and Heme Disassociation Defines Human Hemoglobin Disassembly. Biophysical Journal, 2020, 118, 1381-1400.	0.2	13
225	Electronic structures of active site models for compounds I and II of peroxidase. Journal of the American Chemical Society, 1985, 107, 4013-4015.	6.6	12
226	Enhanced Sampling of Interdomain Motion Using Map-Restrained Langevin Dynamics and NMR: Application to Pin1. Journal of Molecular Biology, 2018, 430, 2164-2180.	2.0	12
227	X.alpha. multiple-scattering study of hexacyanoferrate(III). Inorganic Chemistry, 1981, 20, 528-533.	1.9	11
228	Interpretation of CO/Pt photoemission data via relattvistic cluster calculations. Surface Science, 1981, 106, 523-528.	0.8	11
229	Electronic structure of octachloroditungstate(II). Inorganic Chemistry, 1984, 23, 3271-3273.	1.9	11
230	The Ornsteinâ€“Zernike equation in molecular electronic structure theory. Molecular Physics, 2010, 108, 307-314.	0.8	11
231	Reconciling Structural and Spectroscopic Fingerprints of the Oxygen-Evolving Complex of Photosystem II: A Computational Study of the S₂ State. Journal of Physical Chemistry B, 2018, 122, 11868-11882.	1.2	10
232	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.	1.3	9
233	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.	1.2	9
234	Free energy calculations on the binding of novel thiolactomycin derivatives to E. coli fatty acid synthase I. Bioorganic and Medicinal Chemistry, 2012, 20, 3446-3453.	1.4	8

#	Article	IF	Citations
235	Deleterious effects of carbonâ€“carbon dipolar coupling on RNA NMR dynamics. Journal of Biomolecular NMR, 2020, 74, 321-331.	1.6	8
236	Vectorization of the generalized Born model for molecular dynamics on shared-memory computers. Computational and Theoretical Chemistry, 2001, 549, 193-201.	1.5	7
237	Atomistic Simulations of Heme Dissociation Pathways in Human Methemoglobins Reveal Hidden Intermediates. Biochemistry, 2020, 59, 4093-4107.	1.2	7
238	Using quantum chemistry to estimate chemical shifts in biomolecules. Biophysical Chemistry, 2020, 267, 106476.	1.5	7
239	Theory and applications of the generalized born solvation model in macromolecular simulations. , 2000, 56, 275.		6
240	Coupled intra- and interdomain dynamics support domain cross-talk in Pin1. Journal of Biological Chemistry, 2020, 295, 16585-16603.	1.6	5
241	Integral equation models for solvent in macromolecular crystals. Journal of Chemical Physics, 2022, 156, 014801.	1.2	5
242	Insulatorâ€”conductor transition in tetracyanoplatinate complexes. Chemical Physics Letters, 1982, 91, 353-357.	1.2	4
243	Relativistic molecular orbital theory of zero-field splittings in triplets. Chemical Physics Letters, 1984, 109, 66-70.	1.2	4
244	High-resolution solution structure ofBacillus subtilis IIAglc. , 1998, 31, 258-270.		4
245	Links between the charge model and bonded parameter force constants in biomolecular force fields. Journal of Chemical Physics, 2017, 147, 161730.	1.2	3
246	Refinement of RNA Structures Using Amber Force Fields. Crystals, 2021, 11, 771.	1.0	2
247	Density functional calculations of redox potentials for FeS clusters including solvation effects. Journal of Inorganic Biochemistry, 1993, 51, 449.	1.5	1
248	Analysis of isotropic hyperfine parameters for mononuclear, dinuclear and polynuclear FEî—¸S clusters.. Journal of Inorganic Biochemistry, 1993, 51, 456.	1.5	1
249	NMR Parameters in Proteins and Nucleic Acids. , 2004, , 339-351.		1
250	Molecular underpinnings of integrin binding to collagen-mimetic peptides containing vascular Ehlersâ€“Danlos syndromeâ€“associated substitutions. Journal of Biological Chemistry, 2019, 294, 14442-14453.	1.6	1
251	Simulations of Kindlin-2 PIP binding domains reveal protonation-dependent membrane binding modes. Biophysical Journal, 2021, , .	0.2	1
252	Perspective on "Dynamics of folded proteins". Theoretical Chemistry Accounts, 2000, 103, 332-334.	0.5	0

#	Article	IF	Citations
253	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.	0.2	0