B Montgomery Pettitt

List of Publications by Year
in descending order

159	7,180	71004	71088
papers	citations	43 h-index	80 g-index

168	168	168	4866
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Effects of Flexibility on dsDNAâ€“dsDNA Interactions. Life, 2022, 12, 699.	1.1	1
2	Assessment of the Components of the Electrostatic Potential of Proteins in Solution: Comparing Experiment and Theory. Journal of Physical Chemistry B, 2022, 126, 4543-4554.	1.2	8
3	Quantitative description of a contractile macromolecular machine. Science Advances, 2021, 7, .	4.7	9
4	De novo determination of near-surface electrostatic potentials by NMR. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	26
5	Thermodynamic Compensation in Peptides Following Liquidâ€“Liquid Phase Separation. Journal of Physical Chemistry B, 2021, 125, 6431-6439.	1.2	11
6	Contributions of higher-order proximal distribution functions to solvent structure around proteins. Journal of Chemical Physics, 2021, 155, 104110.	1.2	1
7	Effects of Model Shape, Volume, and Softness of the Capsid for DNA Packaging of phi29. Journal of Physical Chemistry B, 2020, 124, 10337-10344.	1.2	1
8	Dynamics of Ionic Interactions at Proteinâ€“Nucleic Acid Interfaces. Accounts of Chemical Research, 2020, 53, 1802-1810.	7.6	36
9	Structure and the role of filling rate on model dsDNA packed in a phage capsid. Physical Review E, 2020, 101, 012406.	0.8	3
10	Interactions between identical DNA double helices. Physical Review E, 2020, 101, 032414.	0.8	15
11	The lac repressor hinge helix in context: The effect of the DNA binding domain and symmetry. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129538.	1.1	4
12	Physical Chemistry of the Protein Backbone: Enabling the Mechanisms of Intrinsic Protein Disorder. Journal of Physical Chemistry B, 2020, 124, 4379-4390.	1.2	12
13	Tribute to Peter J. Rossky. Journal of Physical Chemistry B, 2020, 124, 10591-10593.	1.2	0
14	Allosteric discrimination at the NADH/ADP regulatory site of glutamate dehydrogenase. Protein Science, 2019, 28, 2080-2088.	3.1	6
15	Mobility of Histidine Side Chains Analyzed with ¹⁵N NMR Relaxation and Cross-Correlation Data: Insight into Zinc-Fingerâ€“DNA Interactions. Journal of Physical Chemistry B, 2019, 123, 3706-3710.	1.2	6
16	Free Energy Calculations Based on Coupling Proximal Distribution Functions and Thermodynamic Cycles. Journal of Chemical Theory and Computation, 2019, 15, 2649-2658.	2.3	3
17	Experimental Evidence of Solvent-Separated Ion Pairs as Metastable States in Electrostatic Interactions of Biological Macromolecules. Journal of Physical Chemistry Letters, 2019, 10, 7937-7941.	2.1	9
18	NMR Methods for Characterizing the Basic Side Chains of Proteins: Electrostatic Interactions, Hydrogen Bonds, and Conformational Dynamics. Methods in Enzymology, 2019, 615, 285-332.	0.4	13

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19	Glutamate dehydrogenase: Structure of a hyperinsulinism mutant, corrections to the atomic model, and insights into a regulatory site. Proteins: Structure, Function and Bioinformatics, 2019, 87, 41-50.	1.5	6
20	Price of disorder in the lac repressor hinge helix. Biopolymers, 2019, 110, e23239.	1.2	4
21	Peptide Solubility Limits: Backbone and Side-Chain Interactions. Journal of Physical Chemistry B, 2018, 122, 3528-3539.	1.2	22
22	Visualizing Individual RuBisCO and Its Assembly into Carboxysomes in Marine Cyanobacteria by Cryo-Electron Tomography. Journal of Molecular Biology, 2018, 430, 4156-4167.	2.0	63
23	Thermodynamics of Conformational Transitions in a Disordered Protein Backbone Model. Biophysical Journal, 2018, 114, 2799-2810.	0.2	14
24	Nonpolar Solvation Free Energy from Proximal Distribution Functions. Journal of Physical Chemistry B, 2017, 121, 3555-3564.	1.2	11
25	Phageâ€like packing structures with mean field sequence dependence. Journal of Computational Chemistry, 2017, 38, 1191-1197.	1.5	7
26	Intramolecular Interactions Overcome Hydration to Drive the Collapse Transition of Gly₁₅. Journal of Physical Chemistry B, 2017, 121, 8078-8084.	1.2	26
27	Optimal updating magnitude in adaptive flat-distribution sampling. Journal of Chemical Physics, 2017, 147, 174105.	1.2	0
28	Influence of DNA sequence on the structure of minicircles under torsional stress. Nucleic Acids Research, 2017, 45, 7633-7642.	6.5	32
29	Accelerating the weighted histogram analysis method by direct inversion in the iterative subspace. Molecular Simulation, 2016, 42, 1079-1089.	0.9	16
30	Protein collapse driven against solvation free energy without <scp>H</scp>â€bonds. Protein Science, 2016, 25, 103-110.	3.1	22
31	Soluteâ€“Solvent Energetics Based on Proximal Distribution Functions. Journal of Physical Chemistry B, 2016, 120, 8230-8237.	1.2	11
32	Importance of disentanglement and entanglement during DNA replication and segregation. Physics of Life Reviews, 2016, 18, 160-164.	1.5	2
33	Solvation Thermodynamics of Oligoglycine with Respect to Chain Length and Flexibility. Biophysical Journal, 2016, 111, 756-767.	0.2	12
34	Reconciling the understanding of â€˜hydrophobicityâ€™ with physics-based models of proteins. Journal of Physics Condensed Matter, 2016, 28, 083003.	0.7	17
35	DNA Shape versus Sequence Variations in the Protein Binding Process. Biophysical Journal, 2016, 110, 534-544.	0.2	7
36	Sequence Affects the Cyclization of DNA Minicircles. Journal of Physical Chemistry Letters, 2016, 7, 1042-1046.	2.1	11

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37	Importance of Hydrophilic Hydration and Intramolecular Interactions in the Thermodynamics of Helixâ€“Coil Transition and Helixâ€“Helix Assembly in a Deca-Alanine Peptide. Journal of Physical Chemistry B, 2016, 120, 69-76.	1.2	26
38	Solubility Limits in Lennard-Jones Mixtures: Effects of Disparate Molecule Geometries. Journal of Physical Chemistry B, 2015, 119, 9450-9459.	1.2	1
39	Dynamic Equilibria of Short-Range Electrostatic Interactions at Molecular Interfaces of Proteinâ€“DNA Complexes. Journal of Physical Chemistry Letters, 2015, 6, 2733-2737.	2.1	39
40	Force fieldâ€dependent solution properties of glycine oligomers. Journal of Computational Chemistry, 2015, 36, 1275-1285.	1.5	26
41	Effects of Acids, Bases, and Heteroatoms on Proximal Radial Distribution Functions for Proteins. Journal of Chemical Theory and Computation, 2015, 11, 1399-1409.	2.3	12
42	Twist-Induced Defects of the P-SSP7 Genome Revealed by Modeling the Cryo-EM Density. Journal of Physical Chemistry B, 2015, 119, 4937-4943.	1.2	7
43	Controlling microarray DNA hybridization efficiency by probe-surface distance and external surface electrostatics. AIP Conference Proceedings, 2015, , .	0.3	2
44	Computation of virial coefficients from integral equations. Journal of Chemical Physics, 2015, 142, 214110.	1.2	5
45	Examining the Assumptions Underlying Continuum-Solvent Models. Journal of Chemical Theory and Computation, 2015, 11, 4593-4600.	2.3	18
46	Solvation and cavity occupation in biomolecules. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 923-931.	1.1	7
47	Secondary Analysis of the NCI-60 Whole Exome Sequencing Data Indicates Significant Presence of Propionibacterium acnes Genomic Material in Leukemia (RPMI-8226) and Central Nervous System (SF-295, SF-539, and SNB-19) Cell Lines. PLoS ONE, 2015, 10, e0127799.	1.1	1
48	Multibody correlations in the hydrophobic solvation of glycine peptides. Journal of Chemical Physics, 2014, 141, 22D525.	1.2	14
49	Modeling DNA Thermodynamics under Torsional Stress. Biophysical Journal, 2014, 106, 1182-1193.	0.2	12
50	A Cavity Corrected 3D-RISM Functional for Accurate Solvation Free Energies. Journal of Chemical Theory and Computation, 2014, 10, 934-941.	2.3	128
51	Computation of high-order virial coefficients in high-dimensional hard-sphere fluids by Mayer sampling. Molecular Physics, 2014, 112, 1427-1447.	0.8	44
52	Conditional Solvation Thermodynamics of Isoleucine in Model Peptides and the Limitations of the Group-Transfer Model. Journal of Physical Chemistry B, 2014, 118, 4080-4087.	1.2	15
53	Solubility and Aggregation of Gly₅ in Water. Journal of Physical Chemistry B, 2014, 118, 9565-9572.	1.2	40
54	Effects of geometry and chemistry on hydrophobic solvation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 14681-14686.	3.3	62

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55	The unsolved â€œsolved-problemâ€•of protein folding. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1024-1027.	2.0	14
56	Communication: Origin of the contributions to DNA structure in phages. Journal of Chemical Physics, 2013, 138, 071103.	1.2	8
57	Solvation Free Energies of Alanine Peptides: The Effect of Flexibility. Journal of Physical Chemistry B, 2013, 117, 16428-16435.	1.2	27
58	Proximal distributions from angular correlations: A measure of the onset of coarse-graining. Journal of Chemical Physics, 2013, 139, 214111.	1.2	4
59	Bullied no more: when and how DNA shoves proteins around. Quarterly Reviews of Biophysics, 2012, 45, 257-299.	2.4	75
60	Peptide Conformational Preferences in Osmolyte Solutions: Transfer Free Energies of Decaalanine. Journal of the American Chemical Society, 2011, 133, 1849-1858.	6.6	121
61	The Binding Process of a Nonspecific Enzyme with DNA. Biophysical Journal, 2011, 101, 1139-1147.	0.2	30
62	Fast Calculations of Electrostatic Solvation Free Energy from Reconstructed Solvent Density Using Proximal Radial Distribution Functions. Journal of Physical Chemistry Letters, 2011, 2, 1626-1632.	2.1	20
63	Note: On the universality of proximal radial distribution functions of proteins. Journal of Chemical Physics, 2011, 134, 106101.	1.2	23
64	Free energy considerations for nucleic acids with dangling ends near a surface: a coarse grained approach. Journal of Physics Condensed Matter, 2011, 23, 325101.	0.7	5
65	Accurate Prediction of Binding Thermodynamics for DNA on Surfaces. Journal of Physical Chemistry B, 2011, 115, 13300-13303.	1.2	24
66	Ion and Solvent Density Distributions around Canonical B-DNA from Integral Equations. Journal of Physical Chemistry B, 2011, 115, 547-556.	1.2	42
67	Integral Equations in the Study of Polar and Ionic Interaction Site Fluids. Journal of Statistical Physics, 2011, 145, 441-466.	0.5	17
68	Electrostatic solvation free energy of amino acid side chain analogs: Implications for the validity of electrostatic linear response in water. Journal of Computational Chemistry, 2011, 32, 878-885.	1.5	27
69	TrimethylamineNâ€oxide influence on the backbone of proteins: An oligoglycine model. Proteins: Structure, Function and Bioinformatics, 2010, 78, 695-704.	1.5	85
70	Protein solvation from theory and simulation: Exact treatment of Coulomb interactions in three-dimensional theories. Journal of Chemical Physics, 2010, 132, 064106.	1.2	69
71	The Behavior of Ions near a Charged Wallâ€”Dependence on Ion Size, Concentration, and Surface Charge.. Journal of Physical Chemistry B, 2010, 114, 6074-6083.	1.2	47
72	A model for structure and thermodynamics of ssDNA and dsDNA near a surface: A coarse grained approach. Computer Physics Communications, 2010, 181, 2001-2007.	3.0	62

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73	Backbone additivity in the transfer model of protein solvation. Protein Science, 2010, 19, 1011-1022.	3.1	71
74	1TP3-07 Peptide conformational preferences in different solutions analyzed by transfer free energy calculations(The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S35.	0.0	0
75	In the absence of writhe, DNA relieves torsional stress with localized, sequence-dependent structural failure to preserve B-form. Nucleic Acids Research, 2009, 37, 5568-5577.	6.5	61
76	Integral Equation Study of the Hydrophobic Interaction between Graphene Plates. Journal of Chemical Theory and Computation, 2008, 4, 1928-1939.	2.3	29
77	Free Energy Calculations for DNA Near Surfaces Using an Ellipsoidal Geometry. Communications in Computational Physics, 2008, 3, 1117-1131.	0.7	7
78	Optimized theory for simple and molecular fluids. Journal of Chemical Physics, 2007, 126, 124107.	1.2	13
79	Molecular Basis of the Apparent Near Ideality of Urea Solutions. Biophysical Journal, 2007, 93, 3392-3407.	0.2	67
80	Thermodynamic Aspects. Advances in Chemical Physics, 2007, , 175-190.	0.3	0
81	Experimental Comparisons and Analysis. Advances in Chemical Physics, 2007, , 191-224.	0.3	0
82	Protein Structure and Dynamics-An Overview. Advances in Chemical Physics, 2007, , 7-21.	0.3	9
83	Potential Functions. Advances in Chemical Physics, 2007, , 23-31.	0.3	1
84	Dynamical Simulation Methods. Advances in Chemical Physics, 2007, , 33-58.	0.3	4
85	Thermodynamic Methods. Advances in Chemical Physics, 2007, , 59-74.	0.3	0
86	Atom and Sidechain Motions. Advances in Chemical Physics, 2007, , 75-116.	0.3	0
87	Rigid-Body Motions. Advances in Chemical Physics, 2007, , 117-126.	0.3	2
88	Larger-Scale Motions. Advances in Chemical Physics, 2007, , 127-136.	0.3	0
89	Solvent Influence on Protein Dynamics. Advances in Chemical Physics, 2007, , 137-174.	0.3	2
90	Enthalpyâ^'Entropy Contributions to the Potential of Mean Force of Nanoscopic Hydrophobic Solutes. Journal of Physical Chemistry B, 2006, 110, 8459-8463.	1.2	133

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91	Electrostatics of DNAâ€“DNA juxtapositions: consequences for type II topoisomerase function. Journal of Physics Condensed Matter, 2006, 18, S173-S185.	0.7	18
92	Solvent participation in Serratia marcescens endonuclease complexes. Proteins: Structure, Function and Bioinformatics, 2005, 62, 982-995.	1.5	11
93	Dynamics of Water Trapped between Hydrophobic Solutes. Journal of Physical Chemistry B, 2005, 109, 6422-6429.	1.2	160
94	Local density profiles are coupled to solute size and attractive potential for nanoscopic hydrophobic solutes. Molecular Simulation, 2005, 31, 457-463.	0.9	36
95	On the Mechanism of Hydrophobic Association of Nanoscopic Solutes. Journal of the American Chemical Society, 2005, 127, 3556-3567.	6.6	284
96	A Non-Watsonâ€“Crick Motif of Base-pairing on Surfaces for Untethered Oligonucleotides. Molecular Simulation, 2004, 30, 121-129.	0.9	14
97	Computationally useful bridge diagram series. III. Lennard-Jones mixtures. Journal of Chemical Physics, 2002, 116, 9413-9421.	1.2	14
98	Solvation and Hydration of Proteins and Nucleic Acids:â€‰ A Theoretical View of Simulation and Experiment. Accounts of Chemical Research, 2002, 35, 376-384.	7.6	321
99	Computationally useful bridge diagram series. II. Diagrams inh-bonds. Journal of Chemical Physics, 2002, 116, 9404-9412.	1.2	25
100	Fine-tuning function: Correlation of hinge domain interactions with functional distinctions between LacI and PurR. Protein Science, 2002, 11, 778-794.	3.1	40
101	A reexamination of virial coefficients of the Lennard-Jones fluid. Theoretical Chemistry Accounts, 2001, 105, 244-251.	0.5	17
102	A study of DNA tethered to a surface by an all-atom molecular dynamics simulation. Theoretical Chemistry Accounts, 2001, 106, 233-235.	0.5	54
103	Simulations of the bis-penicillamine enkephalin in sodium chloride solution: A parameter study. Biopolymers, 2001, 60, 134-152.	1.2	9
104	Structural basis for the activity of pp60c-srcprotein tyrosine kinase inhibitors. Biopolymers, 2001, 59, 167-179.	1.2	2
105	Hydration effects on the electrostatic potential around tuftsin. , 1999, 50, 133-143.		4
106	Structure and dynamics of ?-MSH using DRISM integral equation theory and stochastic dynamics. , 1999, 50, 255-272.		17
107	Sodium and Chlorine Ions as Part of the DNA Solvation Shell. Biophysical Journal, 1999, 77, 1769-1781.	0.2	211
108	A comparison between simulation and poisson-boltzmann fields. , 1999, , .		2

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109	A molecular simulation picture of DNA hydration around A- and B-DNA. , 1998, 48, 199.		94
110	Reconstructing the proteinâ€“water interface. Biopolymers, 1998, 45, 469-478.	1.2	64
111	Diffusion of Solvent around Biomolecular Solutes: A Molecular Dynamics Simulation Study. Biophysical Journal, 1998, 75, 150-158.	0.2	149
112	Comparison of Simulated and Experimentally Determined Dynamics for a Variant of the LacI DNA-Binding Domain, Nlac-P. Biophysical Journal, 1998, 74, 413-421.	0.2	23
113	NMR and quenched molecular dynamics studies of superpotent linear and cyclic Î±â€melanotropins. Chemical Biology and Drug Design, 1998, 51, 420-431.	1.2	27
114	Reconstructing the proteinâ€“water interface. , 1998, 45, 469.		2
115	On the Presence of Rotational Ewald Artifacts in the Equilibrium and Dynamical Properties of a Zwitterionic Tetrapeptide in Aqueous Solution. Journal of Physical Chemistry B, 1997, 101, 3886-3890.	1.2	46
116	Grand canonical ensemble molecular dynamics simulations: Reformulation of extended system dynamics approaches. Journal of Chemical Physics, 1997, 107, 8594-8610.	1.2	69
117	Experiment vs Force Fields:Â DNA Conformation from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 1997, 101, 7361-7363.	1.2	75
118	Computationally useful bridge diagram series for the structure and thermodynamics of Lennard-Jones fluids. Theoretical Chemistry Accounts, 1997, 96, 61-70.	0.5	16
119	A simple two-dimensional representation for the common secondary structural elements of polypeptides and proteins. , 1997, 27, 227-233.		7
120	Modeling the DNA-solvent interface. Biopolymers, 1997, 41, 107-119.	1.2	28
121	Modeling the DNA-solvent interface. , 1997, 41, 107.		2
122	B to A Transition of DNA on the Nanosecond Time Scale. The Journal of Physical Chemistry, 1996, 100, 2564-2566.	2.9	83
123	Salting in Peptides:Â Conformationally Dependent Solubilities and Phase Behavior of a Tripeptide Zwitterion in Electrolyte Solution. Journal of the American Chemical Society, 1996, 118, 1164-1172.	6.6	28
124	Ewald artifacts in liquid state molecular dynamics simulations. Journal of Chemical Physics, 1996, 105, 4289-4293.	1.2	95
125	Dependence of Hydration Free Energy on Solute Size. The Journal of Physical Chemistry, 1996, 100, 1323-1329.	2.9	29
126	Solvent effects on model d(CGÂ·G)7and d(TAÂ·T)7DNA triple helices. Biopolymers, 1995, 35, 457-473.	1.2	15

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127	Conformational states governing the rates of spontaneous transition mutations. Biopolymers, 1995, 36, 169-179.	1.2	7
128	Structure and dynamics of the water around myoglobin. Protein Science, 1995, 4, 149-158.	3.1	73
129	Simulations of conformers of tuftsin and a cyclic tuftsin analog. International Journal of Peptide and Protein Research, 1995, 46, 372-380.	0.1	12
130	Ideal chemical potential contribution in molecular dynamics simulations of the grand canonical ensemble. Molecular Physics, 1994, 82, 897-912.	0.8	46
131	A Connected-cluster of hydration around myoglobin: Correlation between molecular dynamics simulations and experiment. Proteins: Structure, Function and Bioinformatics, 1994, 18, 133-147.	1.5	109
132	Distribution function implied dynamics versus residence times and correlations: Solvation shells of myoglobin. Proteins: Structure, Function and Bioinformatics, 1994, 18, 148-160.	1.5	81
133	Investigations into the common ion effect. Journal of Chemical Physics, 1994, 101, 5093-5109.	1.2	13
134	Molecular recognition of watson-crick base-pair reversals in triple-helix formation: Use of nonnatural oligonucleotide bases. Biopolymers, 1993, 33, 1317-1325.	1.2	9
135	Dynamic simulations of water at constant chemical potential. Journal of Chemical Physics, 1992, 96, 1333-1342.	1.2	65
136	A siteâ€“site theory for finite concentration saline solutions. Journal of Chemical Physics, 1992, 97, 7656-7666.	1.2	273
137	On the correlation between like ion pairs in water. Journal of Chemical Physics, 1992, 96, 4046-4047.	1.2	65
138	Amino acid side-chain populations in aqueous and saline solution: Bis-penicillamine enkephalin. Biopolymers, 1992, 32, 1623-1629.	1.2	17
139	A dielectrically consistent interaction site theory for solventâ€”electrolyte mixtures. Chemical Physics Letters, 1992, 190, 626-630.	1.2	195
140	Molecular dynamics with a variable number of molecules. Molecular Physics, 1991, 72, 169-175.	0.8	100
141	Grand Molecular Dynamics: A Method for Open Systems. Molecular Simulation, 1991, 6, 5-26.	0.9	86
142	Convergence of the Chemical Potential in Aqueous simulations. Molecular Simulation, 1991, 6, 1-4.	0.9	43
143	A method for modeling icosahedral virions: Rotational symmetry boundary conditions. Journal of Computational Chemistry, 1991, 12, 627-634.	1.5	29
144	Peptides in ionic solutions: A comparison of the Ewald and switching function techniques. Journal of Chemical Physics, 1991, 95, 8430-8441.	1.2	156

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145	A study of model energetics and conformational properties of polynucleotide triplexes. Biopolymers, 1990, 30, 517-532.	1.2	16
146	Flexibility of tripeptides in solution: free energy molecular mechanics. International Journal of Peptide and Protein Research, 1990, 35, 315-327.	0.1	15
147	Water under high pressure. Molecular Physics, 1988, 64, 325-336.	0.8	46
148	A theory of the interionic structure of graphite intercalation synthetic metals: Variations with respect to interactions and state. Journal of Chemical Physics, 1988, 89, 1042-1048.	1.2	18
149	A theoretical study of the inclusion complexes of Î²â€quinol. Journal of Chemical Physics, 1988, 89, 968-974.	1.2	8
150	Molecular Dynamics of Coat Proteins of the Human Rhinovirus. Molecular Simulation, 1988, 1, 385-398.	0.9	5
151	Conformations of the glycine dipeptide. Biopolymers, 1987, 26, 1817-1831.	1.2	30
152	Alkali halides in water: Ionâ€“solvent correlations and ionâ€“ion potentials of mean force at infinite dilution. Journal of Chemical Physics, 1986, 84, 5836-5844.	1.2	520
153	New Approaches to Solventâ€Mediated Molecular Interactions. Israel Journal of Chemistry, 1986, 27, 156-162.	1.0	6
154	The interionic potential of mean force in a molecular polar solvent from an extended RISM equation. Journal of Chemical Physics, 1983, 78, 4133-4144.	1.2	255
155	The contribution of hydrogen bonding to the structure of liquid methanol. Journal of Chemical Physics, 1983, 78, 7296-7299.	1.2	60
156	The coupling of long and short range correlations in ISM liquids. Molecular Physics, 1983, 50, 1263-1271.	0.8	60
157	Application of an extended RISM equation to dipolar and quadrupolar fluids. Journal of Chemical Physics, 1982, 77, 509-520.	1.2	290
158	Integral equation predictions of liquid state structure for waterlike intermolecular potentials. Journal of Chemical Physics, 1982, 77, 1451-1457.	1.2	268
159	Theoretical compton profile anisotropics in molecules and solids. VIII. Vibrational, rotational, and temperature-dependent diatomic alkali halide anisotropics. International Journal of Quantum Chemistry, 1980, 18, 697-706.	1.0	0