Jonathan D Hirst

List of Publications by Year
in descending order

169	5,657	66343	102487
papers	citations	42 h-index	66 g-index

191	191	191	5778
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Kernel Methods for Predicting Yields of Chemical Reactions. Journal of Chemical Information and Modeling, 2022, 62, 2077-2092.	5.4	27
2	Effect of Oriented Electric Fields on Biologically Relevant Ironâ€“Sulfur Clusters: Tuning Redox Reactivity for Catalysis. Journal of Chemical Information and Modeling, 2022, , .	5.4	4
3	Alchemical Free Energy Methods Applied to Complexes of the First Bromodomain of BRD4. Journal of Chemical Information and Modeling, 2022, 62, 1458-1470.	5.4	8
4	Software tools for green and sustainable chemistry. Current Opinion in Green and Sustainable Chemistry, 2022, 35, 100623.	5.9	4
5	Daniel Douglas Eley. 1 October 1914â€”3 September 2015. Biographical Memoirs of Fellows of the Royal Society, 2022, 73, 227-249.	0.1	0
6	Structureâ€“Property Relationships in Amorphous Thieno[3,2-b]thiopheneâ€“Diketopyrrolopyrroleâ€“Thiophene-Containing Polymers. Journal of Physical Chemistry C, 2022, 126, 10842-10854.	3.1	5
7	Influence of structure and solubility of chain transfer agents on the RAFT control of dispersion polymerisation in scCO₂. Chemical Science, 2021, 12, 1016-1030.	7.4	4
8	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. Molecules, 2021, 26, 396.	3.8	2
9	Structural variation of proteinâ€“ligand complexes of the first bromodomain of BRD4. Organic and Biomolecular Chemistry, 2021, 19, 5632-5641.	2.8	6
10	Benzene, Toluene, and Monosubstituted Derivatives: Diabatic Nature of the Oscillator Strengths of S₁â†•S₀Transitions. Journal of Physical Chemistry A, 2021, 125, 5237-5245.	2.5	3
11	Memorial Viewpoint for Nicholas A. Besley. Journal of Physical Chemistry A, 2021, 125, 8345-8346.	2.5	1
12	Machine-Learning-Enabled Virtual Screening for Inhibitors of Lysine-Specific Histone Demethylase 1. Molecules, 2021, 26, 7492.	3.8	3
13	A Machine Learning Protocol for Predicting Protein Infrared Spectra. Journal of the American Chemical Society, 2020, 142, 19071-19077.	13.7	55
14	Interaction of the maturation protein of the bacteriophage MS2 and the sex pilus of the Escherichia coli F plasmid. Journal of Molecular Graphics and Modelling, 2020, 101, 107723.	2.4	2
15	Origin of Selectivity in Protein Hydrolysis by Zr(IV)-Containing Metal Oxides as Artificial Proteases. ACS Catalysis, 2020, 10, 13455-13467.	11.2	13
16	Molecular Simulation of Î±vÎ²6 Integrin Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 5487-5498.	5.4	7
17	MÃ¶bius and HÃ¼ckel Cyclacenes with Dewar and Ladenburg Defects. Journal of Physical Chemistry A, 2020, 124, 5408-5414.	2.5	10
18	Unfolding Dynamics of a Photoswitchable Helical Peptide. Journal of Physical Chemistry B, 2020, 124, 5380-5392.	2.6	3

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19	Lateâ€Stage Functionalization by Chanâ€“Lam Amination: Rapid Access to Potent and Selective Integrin Inhibitors. Chemistry - A European Journal, 2020, 26, 7678-7684.	3.3	12
20	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
21	Force Fields for Macromolecular Assemblies Containing Diketopyrrolopyrrole and Thiophene. Journal of Chemical Theory and Computation, 2020, 16, 5150-5162.	5.3	9
22	Dewar Benzenoids Discovered In Carbon Nanobelts. Journal of Physical Chemistry Letters, 2020, 11, 3769-3772.	4.6	13
23	Computed optical spectra of SARS-CoV-2 proteins. Chemical Physics Letters, 2020, 758, 137935.	2.6	13
24	Chapter 7. Machine Learning for Chemical Synthesis. RSC Theoretical and Computational Chemistry Series, 2020, , 169-194.	0.7	4
25	Impact of the Conformational Variability of Oligopeptides on the Computational Prediction of Their CD Spectra. Journal of Physical Chemistry B, 2019, 123, 6694-6704.	2.6	7
26	Electronic Circular Dichroism Spectroscopy of Proteins. CheM, 2019, 5, 2751-2774.	11.7	100
27	Time resolved transient circular dichroism spectroscopy using synchrotron natural polarization. Structural Dynamics, 2019, 6, 054307.	2.3	14
28	Active Search for Computerâ€aided Drug Design. Molecular Informatics, 2018, 37, 1700130.	2.5	17
29	DichroCalc: Improvements in Computing Protein Circular Dichroism Spectroscopy in the Near-Ultraviolet. Journal of Molecular Biology, 2018, 430, 2196-2202.	4.2	21
30	Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica. ACS Biomaterials Science and Engineering, 2018, 4, 4036-4050.	5.2	15
31	Protein Circular Dichroism: Theoretical Aspects. , 2018, , 1-3.		0
32	Simulating Biomolecules: Festschrift to commemorate the 60th birthday of Charles L. Brooks III. Journal of Computational Chemistry, 2017, 38, 1111-1113.	3.3	0
33	Quantitative first principles calculations of protein circular dichroism in the near-ultraviolet. Chemical Science, 2017, 8, 4318-4333.	7.4	28
34	Quantum chemical calculations of tryptophan â†' heme electron and excitation energy transfer rates in myoglobin. Journal of Computational Chemistry, 2017, 38, 1495-1502.	3.3	16
35	Examining the role of protein structural dynamics in drug resistance in Mycobacterium tuberculosis. Chemical Science, 2017, 8, 8384-8399.	7.4	19
36	Computing infrared spectra of proteins using the exciton model. Journal of Computational Chemistry, 2017, 38, 1362-1375.	3.3	23

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37	Probing Polyoxometalateâ€“Protein Interactions Using Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 15280-15289.	3.3	50
38	Probing Polyoxometalate-Protein Interactions Using Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 15157-15157.	3.3	1
39	Docking and molecular dynamics simulations of the ternary complex nisin2:lipid II. Scientific Reports, 2016, 6, 21185.	3.3	16
40	Simulation of Two-Dimensional Infrared Spectroscopy of Peptides Using Localized Normal Modes. Journal of Chemical Theory and Computation, 2016, 12, 1905-1918.	5.3	20
41	Dynamics of chemical bond: general discussion. Faraday Discussions, 2015, 177, 121-154.	3.2	8
42	Local and Global Dynamics: general discussion. Faraday Discussions, 2015, 177, 381-403.	3.2	0
43	Vibronic structure in the far-UV electronic circular dichroism spectra of proteins. Faraday Discussions, 2015, 177, 329-344.	3.2	11
44	Time and Space resolved Methods: general discussion. Faraday Discussions, 2015, 177, 263-292.	3.2	1
45	Accelerating electrostatic pair methods on graphical processing units to study molecules in supercritical carbon dioxide. Faraday Discussions, 2014, 169, 343-357.	3.2	3
46	A theoretical study of the activity in Rh-catalysed hydroformylation: the origin of the enhanced activity of the Ï€-acceptor phosphinine ligand. Catalysis Science and Technology, 2014, 4, 979-987.	4.1	30
47	New CHARMM force field parameters for dehydrated amino acid residues, the key to lantibiotic molecular dynamics simulations. RSC Advances, 2014, 4, 48621-48631.	3.6	13
48	Molecular simulations and visualization: introduction and overview. Faraday Discussions, 2014, 169, 9-22.	3.2	38
49	Studying Biomacromolecules with Two-Dimensional Infrared Spectroscopy. Advances in Protein Chemistry and Structural Biology, 2013, 93, 1-36.	2.3	4
50	Cooperativity and Site Selectivity in the Ileal Lipid Binding Protein. Biochemistry, 2013, 52, 4723-4733.	2.5	12
51	Transformation of the dihedral corrective map for d-amino residues using the CHARMM force field. Chemical Physics Letters, 2012, 543, 142-147.	2.6	1
52	Calculation of Partition Functions and Free Energies of a Binary Mixture Using the Energy Partitioning Method: Application to Carbon Dioxide and Methane. Journal of Physical Chemistry B, 2012, 116, 4535-4542.	2.6	21
53	Structural Insights into the Two Sequential Folding Transition States of the PB1 Domain of NBR1 from Î¦ Value Analysis and Biased Molecular Dynamics Simulations. Biochemistry, 2011, 50, 125-135.	2.5	3
54	Modeling the Infrared and Circular Dichroism Spectroscopy of a Bridged Cyclic Diamide. Journal of Physical Chemistry B, 2011, 115, 5526-5535.	2.6	16

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55	Molecular simulation of the binary mixture of 1â€“1â€“1â€“2â€“tetrafluoroethane and carbon dioxide. Physical Chemistry Chemical Physics, 2011, 13, 15708.	2.8	4
56	Di-8-ANEPPS Emission Spectra in Phospholipid/Cholesterol Membranes: A Theoretical Study. Journal of Physical Chemistry B, 2011, 115, 4160-4167.	2.6	50
57	Comparison of implicit solvent models and force fields in molecular dynamics simulations of the PB1 domain. Chemical Physics Letters, 2011, 515, 283-289.	2.6	5
58	Molecular dynamics simulations and in silico peptide ligand screening of the Elk-1 ETS domain. Journal of Cheminformatics, 2011, 3, 49.	6.1	7
59	Molecular Dynamics Simulations Using Graphics Processing Units. Molecular Informatics, 2011, 30, 498-504.	2.5	23
60	Water order profiles on phospholipid/cholesterol membrane bilayer surfaces. Journal of Computational Chemistry, 2011, 32, 2613-2618.	3.3	16
61	Rapid calculation of partition functions and free energies of fluids. Journal of Chemical Physics, 2011, 135, 174105.	3.0	27
62	First principles predictions of thermophysical properties of refrigerant mixtures. Journal of Chemical Physics, 2011, 134, 114518.	3.0	5
63	Topical perspectives. Journal of Molecular Graphics and Modelling, 2010, 29, 115.	2.4	0
64	A learning classifier system with mutual-information-based fitness. Evolutionary Intelligence, 2010, 3, 31-50.	3.6	8
65	Molecular docking and QSAR of aplyronine A and analogues: potent inhibitors of actin. Journal of Computer-Aided Molecular Design, 2010, 24, 1-15.	2.9	12
66	Automatic structure classification of small proteins using random forest. BMC Bioinformatics, 2010, 11, 364.	2.6	23
67	Predicting Î²-turns and their types using predicted backbone dihedral angles and secondary structures. BMC Bioinformatics, 2010, 11, 407.	2.6	38
68	The JMGM/MGMS graphics prize. Journal of Molecular Graphics and Modelling, 2010, 29, 1.	2.4	0
69	Simulation of Two Dimensional Ultraviolet (2DUV) Spectroscopy of Amyloid Fibrils. Nature Precedings, 2010, , .	0.1	0
70	Stereoselective Disulfide Formation Stabilizes the Local Peptide Conformation in Nisin Mimics. Biochemistry, 2010, 49, 9594-9603.	2.5	8
71	Assembly Pathway of a Designed Î±-Helical Protein Fiber. Biophysical Journal, 2010, 98, 1668-1676.	0.5	57
72	Ultraviolet Spectroscopy of Protein Backbone Transitions in Aqueous Solution: Combined QM and MM Simulations. Journal of Physical Chemistry B, 2010, 114, 8270-8277.	2.6	58

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73	Simulation Study of Chiral Two-Dimensional Ultraviolet Spectroscopy of the Protein Backbone. Journal of the American Chemical Society, 2010, 132, 7769-7775.	13.7	39
74	Gibbs Ensemble Monte Carlo Simulations of Binary Mixtures of Methane, Difluoromethane, and Carbon Dioxide. Journal of Physical Chemistry B, 2010, 114, 3879-3886.	2.6	21
75	Simulation of Two-Dimensional Ultraviolet Spectroscopy of Amyloid Fibrils. Journal of Physical Chemistry B, 2010, 114, 12150-12156.	2.6	20
76	Microscopic structure of liquid 1-1-1-2-tetrafluoroethane (R134a) from Monte Carlo simulation. Physical Chemistry Chemical Physics, 2010, 12, 13266.	2.8	11
77	DichroCalcâ€"circular and linear dichroism online. Bioinformatics, 2009, 25, 539-540.	4.1	111
78	Prediction of backbone dihedral angles and protein secondary structure using support vector machines. BMC Bioinformatics, 2009, 10, 437.	2.6	52
79	Automated Alphabet Reduction for Protein Datasets. BMC Bioinformatics, 2009, 10, 6.	2.6	54
80	Prediction of topological contacts in proteins using learning classifier systems. Soft Computing, 2009, 13, 245-258.	3.6	27
81	Exploring protein structural dissimilarity to facilitate structure classification. BMC Structural Biology, 2009, 9, 60.	2.3	0
82	Interpretable correlation descriptors for quantitative structure-activity relationships. Journal of Cheminformatics, 2009, 1, 22.	6.1	16
83	Supervised machine learning algorithms for protein structure classification. Computational Biology and Chemistry, 2009, 33, 216-223.	2.3	77
84	Electronic structure and circular dichroism spectroscopy of naphthalenediimide nanotubes. Physical Chemistry Chemical Physics, 2009, 11, 6060.	2.8	32
85	Electronic Structure of 5-Hydroxyindole: From Gas Phase to Explicit Solvation. Journal of Physical Chemistry B, 2009, 113, 2535-2541.	2.6	33
86	Flow Linear Dichroism of Some Prototypical Proteins. Journal of the American Chemical Society, 2009, 131, 13305-13314.	13.7	36
87	Calculating the Fluorescence of 5-Hydroxytryptophan in Proteins. Journal of Physical Chemistry B, 2009, 113, 14521-14528.	2.6	17
88	Machine Learning in Virtual Screening. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 332-343.	1.1	169
89	Conformation and dynamics of the threeâ€helix bundle UBA domain of p62 from experiment and simulation. Proteins: Structure, Function and Bioinformatics, 2008, 71, 227-240.	2.6	7
90	Prediction of glycosylation sites using random forests. BMC Bioinformatics, 2008, 9, 500.	2.6	199

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91	Charge-Transfer Transitions in the Vacuum-Ultraviolet of Protein Circular Dichroism Spectra. Journal of Physical Chemistry B, 2008, 112, 1866-1874.	2.6	53
92	Prediction of recursive convex hull class assignments for protein residues. Bioinformatics, 2008, 24, 916-923.	4.1	42
93	Search Strategies in Structural Bioinformatics. Current Protein and Peptide Science, 2008, 9, 260-274.	1.4	13
94	Data Mining in Proteomics with Learning Classifier Systems. Studies in Computational Intelligence, 2008, , 17-46.	0.9	4
95	Automated alphabet reduction method with evolutionary algorithms for protein structure prediction. , 2007, , .		38
96	Circular and linear dichroism of proteins. Physical Chemistry Chemical Physics, 2007, 9, 2020.	2.8	153
97	Contemporary QSAR Classifiers Compared. Journal of Chemical Information and Modeling, 2007, 47, 219-227.	5.4	122
98	Similarity by Compression. Journal of Chemical Information and Modeling, 2007, 47, 25-33.	5.4	15
99	Calculations on the Electronic Excited States of Ureas and Oligoureas. Journal of Physical Chemistry B, 2007, 111, 3274-3279.	2.6	15
100	The Structural Determinants of Macrolide-Actin Binding: In Silico Insights. Biophysical Journal, 2007, 92, 3862-3867.	0.5	6
101	TMACC:â€‰ Interpretable Correlation Descriptors for Quantitative Structureâ^'Activity Relationships. Journal of Chemical Information and Modeling, 2007, 47, 626-634.	5.4	31
102	Statistical Analysis of Unlabeled Point Sets: Comparing Molecules in Chemoinformatics. Biometrics, 2007, 63, 237-251.	1.4	30
103	ProCKSI: a decision support system for Protein (Structure) Comparison, Knowledge, Similarity and Information. BMC Bioinformatics, 2007, 8, 416.	2.6	48
104	Effects of ulapualide A and synthetic macrolide analogues on actin dynamics and gene regulation. Cellular and Molecular Life Sciences, 2007, 64, 487-497.	5.4	17
105	Ab initio study of the toluene dimer. Chemical Physics Letters, 2006, 427, 410-413.	2.6	25
106	First-principles calculations of protein circular dichroism in the far-ultraviolet and beyond. Chirality, 2006, 18, 340-347.	2.6	25
107	Modeling the amide I bands of small peptides. Journal of Chemical Physics, 2006, 125, 044312.	3.0	202
108	Charge-Transfer Transitions in Protein Circular Dichroism Calculations. Journal of the American Chemical Society, 2006, 128, 12414-12415.	13.7	34

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109	Coordination number prediction using learning classifier systems. , 2006, , .		16
110	From HP Lattice Models to Real Proteins: Coordination Number Prediction Using Learning Classifier Systems. Lecture Notes in Computer Science, 2006, , 208-220.	1.3	11
111	PREDICTION OF RESIDUE EXPOSURE AND CONTACT NUMBER FOR SIMPLIFIED HP LATTICE MODEL PROTEINS USING LEARNING CLASSIFIER SYSTEMS. , 2006, , .		3
112	Lattice models of peptide aggregation: Evaluation of conformational search algorithms. Journal of Computational Chemistry, 2005, 26, 1638-1646.	3.3	9
113	Exploring Phase-Transfer Catalysis with Molecular Dynamics and 3D/4D Quantitative Structureâ€"Selectivity Relationships.. ChemInform, 2005, 36, no.	0.0	0
114	Rapid Screening of Cinchona Alkaloid Derived Phase-Transfer Catalysts: Application in the Optimization of a Glycine Imine Alkylation. ChemInform, 2005, 36, no.	0.0	0
115	Protein secondary structure prediction with dihedral angles. Proteins: Structure, Function and Bioinformatics, 2005, 59, 476-481.	2.6	87
116	Population dynamics simulations of functional model proteins. Journal of Chemical Physics, 2005, 123, 154907.	3.0	14
117	Recent Applications of Neural Networks in Bioinformatics. , 2005, , 91-97.		3
118	Theoretical studies of the amide I vibrational frequencies of [Leu]-enkephalin. Molecular Physics, 2005, 103, 1531-1546.	1.7	49
119	Exploring Phase-Transfer Catalysis with Molecular Dynamics and 3D/4D Quantitative Structureâ^'Selectivity Relationships. Journal of Chemical Information and Modeling, 2005, 45, 971-981.	5.4	43
120	Inhibition of the Tyrosine Kinase, Syk, Analyzed by Stepwise Nonparametric Regression. Journal of Chemical Information and Modeling, 2005, 45, 768-776.	5.4	4
121	Modeling the Absorption Spectrum of Tryptophan in Proteins. Journal of Physical Chemistry B, 2005, 109, 23061-23069.	2.6	46
122	Predicting protein secondary structure by cascade-correlation neural networks. Bioinformatics, 2004, 20, 419-420.	4.1	12
123	A Sequential Molecular Mechanics/Quantum Mechanics Study of the Electronic Spectra of Amides. Journal of the American Chemical Society, 2004, 126, 13502-13511.	13.7	68
124	Calculations of protein circular dichroism from first principles. Chirality, 2004, 16, 234-243.	2.6	27
125	Charge-transfer transitions in protein circular dichroism spectra. Computational and Theoretical Chemistry, 2004, 675, 53-60.	1.5	25
126	Computational screening of combinatorial catalyst librariesElectronic supplementary information (ESI) available: predicted and observed e.e. values for the 88 catalysts in the library; full CoMFA parameters; aligned molecular coordinates. See http://www.rsc.org/suppdata/cc/b4/b402378a/. Chemical Communications, 2004, , 1410.	4.1	18

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127	Calculating vibrational frequencies of amides: From formamide to concanavalin A. Physical Chemistry Chemical Physics, 2004, 6, 998-1005.	2.8	25
128	Vibrational analysis of capped [Leu]enkephalin. Physical Chemistry Chemical Physics, 2004, 6, 2580.	2.8	10
129	On the Stability of CoMFA Models. Journal of Chemical Information and Computer Sciences, 2004, 44, 1294-1300.	2.8	22
130	First-Principles Calculations of Protein Circular Dichroism in the Near Ultravioletâ€. Biochemistry, 2004, 43, 11092-11102.	2.5	71
131	Molecular dynamics simulations of a helicase. Proteins: Structure, Function and Bioinformatics, 2003, 52, 254-262.	2.6	11
132	Influence of Electrostatic Environment on the Vibrational Frequencies of Proteins. Journal of Physical Chemistry A, 2003, 107, 6843-6849.	2.5	28
133	Ab Initio Study of Aromatic Side Chains of Amino Acids in Gas Phase and Solution. Journal of Physical Chemistry A, 2003, 107, 11191-11200.	2.5	48
134	Electronic Circular Dichroism of Proteins from First-Principles Calculations. Journal of Physical Chemistry B, 2003, 107, 11813-11819.	2.6	57
135	Influence of Tyrosine on the Electronic Circular Dichroism of Helical Peptides. Journal of Physical Chemistry B, 2003, 107, 8682-8688.	2.6	36
136	Three-dimensional functional model proteins: Structure function and evolution. Journal of Chemical Physics, 2003, 119, 3453-3460.	3.0	20
137	Theoretical studies of time-resolved spectroscopy of protein folding. Faraday Discussions, 2003, 122, 253-267.	3.2	28
138	Density Functional Theory Vibrational Frequencies of Amides and Amide Dimers. Journal of Physical Chemistry A, 2002, 106, 7858-7867.	2.5	74
139	Stabilizing Interactions between Aromatic and Basic Side Chains in Î±-Helical Peptides and Proteins. Tyrosine Effects on Helix Circular Dichroism. Journal of the American Chemical Society, 2002, 124, 12706-12714.	13.7	82
140	Flow oriented linear dichroism to probe protein orientation in membrane environments. Physical Chemistry Chemical Physics, 2002, 4, 4051-4057.	2.8	72
141	Application of Non-Parametric Regression to Quantitative Structureâ€“Activity Relationships. Bioorganic and Medicinal Chemistry, 2002, 10, 1037-1041.	3.0	7
142	Short Hydrogen Bonds, Circular Dichroism, and Over-Estimates of Peptide Helicity We thank BBSRC for financial support (grant 42/B1524).. Angewandte Chemie - International Edition, 2001, 40, 3619.	13.8	18
143	Evolution of functional model proteins. Journal of Chemical Physics, 2001, 115, 1935-1942.	3.0	33
144	Computer Modeling of Protein Structure. , 2001, , .		0

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145	Hydrogen bonding in protein circular dichroism calculations. Computational and Theoretical Chemistry, 2000, 506, 161-167.	1.5	12
146	Electronic Structure of a Rigid Cyclic Diamide. Journal of Physical Chemistry B, 2000, 104, 12371-12377.	2.6	23
147	Nonparametric Regression Applied to Quantitative Structureâ^'Activity Relationships. Journal of Chemical Information and Computer Sciences, 2000, 40, 452-459.	2.8	27
148	The evolutionary landscape of functional model proteins. Protein Engineering, Design and Selection, 1999, 12, 721-726.	2.1	46
149	Theoretical Studies toward Quantitative Protein Circular Dichroism Calculations. Journal of the American Chemical Society, 1999, 121, 9636-9644.	13.7	151
150	Ab Initio Study of the Electronic Spectrum of Formamide with Explicit Solvent. Journal of the American Chemical Society, 1999, 121, 8559-8566.	13.7	87
151	Response to â€œComment on â€˜Improving protein circular dichroism calculations in the far-ultraviolet through reparameterizing the amide chromophoreâ€™â€‰â€•[J. Chem. Phys. 111, 2844 (1999)]. Journal of Chemical Physics, 1999, 111, 2846-2847.	3.0	21
152	Do active site conformations of small ligands correspond to low free-energy solution structures?. Journal of Computer-Aided Molecular Design, 1998, 12, 563-572.	2.9	94
153	Assessing energy functions for flexible docking. Journal of Computational Chemistry, 1998, 19, 1612-1622.	3.3	144
154	Assessing search strategies for flexible docking. Journal of Computational Chemistry, 1998, 19, 1623-1631.	3.3	112
155	Ab Initio Study of the Effect of Solvation on the Electronic Spectra of Formamide andN-Methylacetamide. Journal of Physical Chemistry A, 1998, 102, 10791-10797.	2.5	69
156	Improving protein circular dichroism calculations in the far-ultraviolet through reparametrizing the amide chromophore. Journal of Chemical Physics, 1998, 109, 782-788.	3.0	50
157	Ab InitioCalculations of the Vibrational and Electronic Spectra of Diketopiperazine. Journal of Physical Chemistry A, 1998, 102, 7519-7524.	2.5	32
158	Multireference Configuration Interaction Calculations of Electronic States ofN-Methylformamide, Acetamide, andN-Methylacetamide. Journal of Physical Chemistry A, 1997, 101, 4821-4827.	2.5	63
159	Nonlinear Quantitative Structureâ^'Activity Relationship for the Inhibition of Dihydrofolate Reductase by Pyrimidines. Journal of Medicinal Chemistry, 1996, 39, 3526-3532.	6.4	22
160	Predicting leucine zipper structures from sequence. Protein Engineering, Design and Selection, 1996, 9, 657-662.	2.1	35
161	Ab InitioCalculations of the Excited States of Formamide. The Journal of Physical Chemistry, 1996, 100, 13487-13491.	2.9	40
162	Molecular Dynamics Simulations of Isolated Helixes of Myoglobin. Biochemistry, 1995, 34, 7614-7621.	2.5	78

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163	COMPARISON OF ARTIFICIAL INTELLIGENCE METHODS FOR MODELING PHARMACEUTICAL QSARS. Applied Artificial Intelligence, 1995, 9, 213-233.	3.2	30
164	Quantitative structure-activity relationships by neural networks and inductive logic programming. I. The inhibition of dihydrofolate reductase by pyrimidines. Journal of Computer-Aided Molecular Design, 1994, 8, 405-420.	2.9	61
165	Quantitative structure-activity relationships by neural networks and inductive logic programming. II. The inhibition of dihydrofolate reductase by triazines. Journal of Computer-Aided Molecular Design, 1994, 8, 421-432.	2.9	55
166	Helicity, Circular Dichroism and Molecular Dynamics of Proteins. Journal of Molecular Biology, 1994, 243, 173-178.	4.2	84
167	New approaches to QSAR: Neural networks and machine learning. Journal of Computer - Aided Molecular Design, 1993, 1, 279-290.	1.0	26
168	Prediction of structural and functional features of protein and nucleic acid sequences by artificial neural networks. Biochemistry, 1992, 31, 7211-7218.	2.5	128
169	Quantitative protein circular dichroism calculations. Special Publication - Royal Society of Chemistry, 0, , 20-30.	0.0	0