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	Vibrational Spectroscopic Map, Vibrational Spectroscopy, and Intermolecular Interaction. Chemical Reviews, 2020, 120, 7152-7218.	47.7	205
2	Modeling the amide I bands of small peptides. Journal of Chemical Physics, 2006, 125, 044312.	3.0	202
3	Prediction of glycosylation sites using random forests. BMC Bioinformatics, 2008, 9, 500.	2.6	199
4	Machine Learning in Virtual Screening. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 332-343.	1.1	169
5	Circular and linear dichroism of proteins. Physical Chemistry Chemical Physics, 2007, 9, 2020.	2.8	153
6	Theoretical Studies toward Quantitative Protein Circular Dichroism Calculations. Journal of the American Chemical Society, 1999, 121, 9636-9644.	13.7	151
7	Assessing energy functions for flexible docking. Journal of Computational Chemistry, 1998, 19, 1612-1622.	3.3	144
8	Prediction of structural and functional features of protein and nucleic acid sequences by artificial neural networks. Biochemistry, 1992, 31, 7211-7218.	2.5	128
9	Contemporary QSAR Classifiers Compared. Journal of Chemical Information and Modeling, 2007, 47, 219-227.	5.4	122
10	Assessing search strategies for flexible docking. Journal of Computational Chemistry, 1998, 19, 1623-1631.	3.3	112
11	DichroCalcâ€"circular and linear dichroism online. Bioinformatics, 2009, 25, 539-540.	4.1	111
12	Electronic Circular Dichroism Spectroscopy of Proteins. CheM, 2019, 5, 2751-2774.	11.7	100
13	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
14	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
15	Protein secondary structure prediction with dihedral angles. Proteins: Structure, Function and Bioinformatics, 2005, 59, 476-481.	2.6	87
16	Helicity, Circular Dichroism and Molecular Dynamics of Proteins. Journal of Molecular Biology, 1994, 243, 173-178.	4.2	84
17	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
18	Molecular Dynamics Simulations of Isolated Helixes of Myoglobin. Biochemistry, 1995, 34, 7614-7621.	2.5	78

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19	Supervised machine learning algorithms for protein structure classification. Computational Biology and Chemistry, 2009, 33, 216-223.	2.3	77
20	Density Functional Theory Vibrational Frequencies of Amides and Amide Dimers. Journal of Physical Chemistry A, 2002, 106, 7858-7867.	2.5	74
21	Flow oriented linear dichroism to probe protein orientation in membrane environments. Physical Chemistry Chemical Physics, 2002, 4, 4051-4057.	2.8	72
22	First-Principles Calculations of Protein Circular Dichroism in the Near Ultravioletâ€. Biochemistry, 2004, 43, 11092-11102.	2.5	71
23	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
24	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
25	Multireference Configuration Interaction Calculations of Electronic States ofN-Methylformamide, Acetamide, andN-Methylacetamide. Journal of Physical Chemistry A, 1997, 101, 4821-4827.	2.5	63
26	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
27	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
28	Electronic Circular Dichroism of Proteins from First-Principles Calculations. Journal of Physical Chemistry B, 2003, 107, 11813-11819.	2.6	57
29	Assembly Pathway of a Designed Î±-Helical Protein Fiber. Biophysical Journal, 2010, 98, 1668-1676.	0.5	57
30	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
31	A Machine Learning Protocol for Predicting Protein Infrared Spectra. Journal of the American Chemical Society, 2020, 142, 19071-19077.	13.7	55
32	Automated Alphabet Reduction for Protein Datasets. BMC Bioinformatics, 2009, 10, 6.	2.6	54
33	Charge-Transfer Transitions in the Vacuum-Ultraviolet of Protein Circular Dichroism Spectra. Journal of Physical Chemistry B, 2008, 112, 1866-1874.	2.6	53
34	Prediction of backbone dihedral angles and protein secondary structure using support vector machines. BMC Bioinformatics, 2009, 10, 437.	2.6	52
35	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
36	Di-8-ANEPPS Emission Spectra in Phospholipid/Cholesterol Membranes: A Theoretical Study. Journal of Physical Chemistry B, 2011, 115, 4160-4167.	2.6	50

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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	Theoretical studies of the amide I vibrational frequencies of [Leu]-enkephalin. Molecular Physics, 2005, 103, 1531-1546.	1.7	49
39	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
40	ProCKSI: a decision support system for Protein (Structure) Comparison, Knowledge, Similarity and Information. BMC Bioinformatics, 2007, 8, 416.	2.6	48
41	The evolutionary landscape of functional model proteins. Protein Engineering, Design and Selection, 1999, 12, 721-726.	2.1	46
42	Modeling the Absorption Spectrum of Tryptophan in Proteins. Journal of Physical Chemistry B, 2005, 109, 23061-23069.	2.6	46
43	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
44	Prediction of recursive convex hull class assignments for protein residues. Bioinformatics, 2008, 24, 916-923.	4.1	42
45	Ab InitioCalculations of the Excited States of Formamide. The Journal of Physical Chemistry, 1996, 100, 13487-13491.	2.9	40
46	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
47	Automated alphabet reduction method with evolutionary algorithms for protein structure prediction. , 2007, , .		38
48	Predicting Î²-turns and their types using predicted backbone dihedral angles and secondary structures. BMC Bioinformatics, 2010, 11, 407.	2.6	38
49	Molecular simulations and visualization: introduction and overview. Faraday Discussions, 2014, 169, 9-22.	3.2	38
50	Influence of Tyrosine on the Electronic Circular Dichroism of Helical Peptides. Journal of Physical Chemistry B, 2003, 107, 8682-8688.	2.6	36
51	Flow Linear Dichroism of Some Prototypical Proteins. Journal of the American Chemical Society, 2009, 131, 13305-13314.	13.7	36
52	Predicting leucine zipper structures from sequence. Protein Engineering, Design and Selection, 1996, 9, 657-662.	2.1	35
53	Charge-Transfer Transitions in Protein Circular Dichroism Calculations. Journal of the American Chemical Society, 2006, 128, 12414-12415.	13.7	34
54	Evolution of functional model proteins. Journal of Chemical Physics, 2001, 115, 1935-1942.	3.0	33

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55	Electronic Structure of 5-Hydroxyindole: From Gas Phase to Explicit Solvation. Journal of Physical Chemistry B, 2009, 113, 2535-2541.	2.6	33
56	Ab InitioCalculations of the Vibrational and Electronic Spectra of Diketopiperazine. Journal of Physical Chemistry A, 1998, 102, 7519-7524.	2.5	32
57	Electronic structure and circular dichroism spectroscopy of naphthalenediimide nanotubes. Physical Chemistry Chemical Physics, 2009, 11, 6060.	2.8	32
58	TMACC:â€‰ Interpretable Correlation Descriptors for Quantitative Structureâ^'Activity Relationships. Journal of Chemical Information and Modeling, 2007, 47, 626-634.	5.4	31
59	COMPARISON OF ARTIFICIAL INTELLIGENCE METHODS FOR MODELING PHARMACEUTICAL QSARS. Applied Artificial Intelligence, 1995, 9, 213-233.	3.2	30
60	Statistical Analysis of Unlabeled Point Sets: Comparing Molecules in Chemoinformatics. Biometrics, 2007, 63, 237-251.	1.4	30
61	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
62	Influence of Electrostatic Environment on the Vibrational Frequencies of Proteins. Journal of Physical Chemistry A, 2003, 107, 6843-6849.	2.5	28
63	Theoretical studies of time-resolved spectroscopy of protein folding. Faraday Discussions, 2003, 122, 253-267.	3.2	28
64	Quantitative first principles calculations of protein circular dichroism in the near-ultraviolet. Chemical Science, 2017, 8, 4318-4333.	7.4	28
65	Nonparametric Regression Applied to Quantitative Structureâ^'Activity Relationships. Journal of Chemical Information and Computer Sciences, 2000, 40, 452-459.	2.8	27
66	Calculations of protein circular dichroism from first principles. Chirality, 2004, 16, 234-243.	2.6	27
67	Prediction of topological contacts in proteins using learning classifier systems. Soft Computing, 2009, 13, 245-258.	3.6	27
68	Rapid calculation of partition functions and free energies of fluids. Journal of Chemical Physics, 2011, 135, 174105.	3.0	27
69	Kernel Methods for Predicting Yields of Chemical Reactions. Journal of Chemical Information and Modeling, 2022, 62, 2077-2092.	5.4	27
70	New approaches to QSAR: Neural networks and machine learning. Journal of Computer - Aided Molecular Design, 1993, 1, 279-290.	1.0	26
71	Charge-transfer transitions in protein circular dichroism spectra. Computational and Theoretical Chemistry, 2004, 675, 53-60.	1.5	25
72	Calculating vibrational frequencies of amides: From formamide to concanavalin A. Physical Chemistry Chemical Physics, 2004, 6, 998-1005.	2.8	25

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73	Ab initio study of the toluene dimer. Chemical Physics Letters, 2006, 427, 410-413.	2.6	25
74	First-principles calculations of protein circular dichroism in the far-ultraviolet and beyond. Chirality, 2006, 18, 340-347.	2.6	25
75	Electronic Structure of a Rigid Cyclic Diamide. Journal of Physical Chemistry B, 2000, 104, 12371-12377.	2.6	23
76	Automatic structure classification of small proteins using random forest. BMC Bioinformatics, 2010, 11, 364.	2.6	23
77	Molecular Dynamics Simulations Using Graphics Processing Units. Molecular Informatics, 2011, 30, 498-504.	2.5	23
78	Computing infrared spectra of proteins using the exciton model. Journal of Computational Chemistry, 2017, 38, 1362-1375.	3.3	23
79	Nonlinear Quantitative Structureâ^'Activity Relationship for the Inhibition of Dihydrofolate Reductase by Pyrimidines. Journal of Medicinal Chemistry, 1996, 39, 3526-3532.	6.4	22
80	On the Stability of CoMFA Models. Journal of Chemical Information and Computer Sciences, 2004, 44, 1294-1300.	2.8	22
81	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
82	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
83	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
84	DichroCalc: Improvements in Computing Protein Circular Dichroism Spectroscopy in the Near-Ultraviolet. Journal of Molecular Biology, 2018, 430, 2196-2202.	4.2	21
85	Three-dimensional functional model proteins: Structure function and evolution. Journal of Chemical Physics, 2003, 119, 3453-3460.	3.0	20
86	Simulation of Two-Dimensional Ultraviolet Spectroscopy of Amyloid Fibrils. Journal of Physical Chemistry B, 2010, 114, 12150-12156.	2.6	20
87	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
88	Examining the role of protein structural dynamics in drug resistance in Mycobacterium tuberculosis. Chemical Science, 2017, 8, 8384-8399.	7.4	19
89	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
90	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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91	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
92	Calculating the Fluorescence of 5-Hydroxytryptophan in Proteins. Journal of Physical Chemistry B, 2009, 113, 14521-14528.	2.6	17
93	Active Search for Computerâ€aided Drug Design. Molecular Informatics, 2018, 37, 1700130.	2.5	17
94	Coordination number prediction using learning classifier systems. , 2006, , .		16
95	Interpretable correlation descriptors for quantitative structure-activity relationships. Journal of Cheminformatics, 2009, 1, 22.	6.1	16
96	Modeling the Infrared and Circular Dichroism Spectroscopy of a Bridged Cyclic Diamide. Journal of Physical Chemistry B, 2011, 115, 5526-5535.	2.6	16
97	Water order profiles on phospholipid/cholesterol membrane bilayer surfaces. Journal of Computational Chemistry, 2011, 32, 2613-2618.	3.3	16
98	Docking and molecular dynamics simulations of the ternary complex nisin2:lipid II. Scientific Reports, 2016, 6, 21185.	3.3	16
99	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
100	Similarity by Compression. Journal of Chemical Information and Modeling, 2007, 47, 25-33.	5.4	15
101	Calculations on the Electronic Excited States of Ureas and Oligoureas. Journal of Physical Chemistry B, 2007, 111, 3274-3279.	2.6	15
102	Atomistic Details of Chymotrypsin Conformational Changes upon Adsorption on Silica. ACS Biomaterials Science and Engineering, 2018, 4, 4036-4050.	5.2	15
103	Population dynamics simulations of functional model proteins. Journal of Chemical Physics, 2005, 123, 154907.	3.0	14
104	Time resolved transient circular dichroism spectroscopy using synchrotron natural polarization. Structural Dynamics, 2019, 6, 054307.	2.3	14
105	Search Strategies in Structural Bioinformatics. Current Protein and Peptide Science, 2008, 9, 260-274.	1.4	13
106	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
107	Origin of Selectivity in Protein Hydrolysis by Zr(IV)-Containing Metal Oxides as Artificial Proteases. ACS Catalysis, 2020, 10, 13455-13467.	11.2	13
108	Dewar Benzenoids Discovered In Carbon Nanobelts. Journal of Physical Chemistry Letters, 2020, 11, 3769-3772.	4.6	13

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109	Computed optical spectra of SARS-CoV-2 proteins. Chemical Physics Letters, 2020, 758, 137935.	2.6	13
110	Hydrogen bonding in protein circular dichroism calculations. Computational and Theoretical Chemistry, 2000, 506, 161-167.	1.5	12
111	Predicting protein secondary structure by cascade-correlation neural networks. Bioinformatics, 2004, 20, 419-420.	4.1	12
112	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
113	Cooperativity and Site Selectivity in the Ileal Lipid Binding Protein. Biochemistry, 2013, 52, 4723-4733.	2.5	12
114	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
115	Molecular dynamics simulations of a helicase. Proteins: Structure, Function and Bioinformatics, 2003, 52, 254-262.	2.6	11
116	Microscopic structure of liquid 1-1-1-2-tetrafluoroethane (R134a) from Monte Carlo simulation. Physical Chemistry Chemical Physics, 2010, 12, 13266.	2.8	11
117	Vibronic structure in the far-UV electronic circular dichroism spectra of proteins. Faraday Discussions, 2015, 177, 329-344.	3.2	11
118	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
119	Vibrational analysis of capped [Leu]enkephalin. Physical Chemistry Chemical Physics, 2004, 6, 2580.	2.8	10
120	MÃ¶bius and HÃ¼ckel Cyclacenes with Dewar and Ladenburg Defects. Journal of Physical Chemistry A, 2020, 124, 5408-5414.	2.5	10
121	Lattice models of peptide aggregation: Evaluation of conformational search algorithms. Journal of Computational Chemistry, 2005, 26, 1638-1646.	3.3	9
122	Force Fields for Macromolecular Assemblies Containing Diketopyrrolopyrrole and Thiophene. Journal of Chemical Theory and Computation, 2020, 16, 5150-5162.	5.3	9
123	A learning classifier system with mutual-information-based fitness. Evolutionary Intelligence, 2010, 3, 31-50.	3.6	8
124	Stereoselective Disulfide Formation Stabilizes the Local Peptide Conformation in Nisin Mimics. Biochemistry, 2010, 49, 9594-9603.	2.5	8
125	Dynamics of chemical bond: general discussion. Faraday Discussions, 2015, 177, 121-154.	3.2	8
126	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

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127	Application of Non-Parametric Regression to Quantitative Structureâ€“Activity Relationships. Bioorganic and Medicinal Chemistry, 2002, 10, 1037-1041.	3.0	7
128	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
129	Molecular dynamics simulations and in silico peptide ligand screening of the Elk-1 ETS domain. Journal of Cheminformatics, 2011, 3, 49.	6.1	7
130	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
131	Molecular Simulation of Î±vÎ²6 Integrin Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 5487-5498.	5.4	7
132	The Structural Determinants of Macrolide-Actin Binding: In Silico Insights. Biophysical Journal, 2007, 92, 3862-3867.	0.5	6
133	Structural variation of proteinâ€“ligand complexes of the first bromodomain of BRD4. Organic and Biomolecular Chemistry, 2021, 19, 5632-5641.	2.8	6
134	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
135	First principles predictions of thermophysical properties of refrigerant mixtures. Journal of Chemical Physics, 2011, 134, 114518.	3.0	5
136	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
137	Inhibition of the Tyrosine Kinase, Syk, Analyzed by Stepwise Nonparametric Regression. Journal of Chemical Information and Modeling, 2005, 45, 768-776.	5.4	4
138	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
139	Studying Biomacromolecules with Two-Dimensional Infrared Spectroscopy. Advances in Protein Chemistry and Structural Biology, 2013, 93, 1-36.	2.3	4
140	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
141	Data Mining in Proteomics with Learning Classifier Systems. Studies in Computational Intelligence, 2008, , 17-46.	0.9	4
142	Chapter 7. Machine Learning for Chemical Synthesis. RSC Theoretical and Computational Chemistry Series, 2020, , 169-194.	0.7	4
143	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
144	Software tools for green and sustainable chemistry. Current Opinion in Green and Sustainable Chemistry, 2022, 35, 100623.	5.9	4

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145	Recent Applications of Neural Networks in Bioinformatics. , 2005, , 91-97.		3
146	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
147	Accelerating electrostatic pair methods on graphical processing units to study molecules in supercritical carbon dioxide. Faraday Discussions, 2014, 169, 343-357.	3.2	3
148	Unfolding Dynamics of a Photoswitchable Helical Peptide. Journal of Physical Chemistry B, 2020, 124, 5380-5392.	2.6	3
149	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
150	PREDICTION OF RESIDUE EXPOSURE AND CONTACT NUMBER FOR SIMPLIFIED HP LATTICE MODEL PROTEINS USING LEARNING CLASSIFIER SYSTEMS. , 2006, , .		3
151	Machine-Learning-Enabled Virtual Screening for Inhibitors of Lysine-Specific Histone Demethylase 1. Molecules, 2021, 26, 7492.	3.8	3
152	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
153	Near-Ultraviolet Circular Dichroism and Two-Dimensional Spectroscopy of Polypeptides. Molecules, 2021, 26, 396.	3.8	2
154	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
155	Time and Space resolved Methods: general discussion. Faraday Discussions, 2015, 177, 263-292.	3.2	1
156	Probing Polyoxometalate-Protein Interactions Using Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 15157-15157.	3.3	1
157	Memorial Viewpoint for Nicholas A. Besley. Journal of Physical Chemistry A, 2021, 125, 8345-8346.	2.5	1
158	Exploring Phase-Transfer Catalysis with Molecular Dynamics and 3D/4D Quantitative Structureâ€"Selectivity Relationships.. ChemInform, 2005, 36, no.	0.0	0
159	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
160	Exploring protein structural dissimilarity to facilitate structure classification. BMC Structural Biology, 2009, 9, 60.	2.3	0
161	Topical perspectives. Journal of Molecular Graphics and Modelling, 2010, 29, 115.	2.4	0
162	The JMGM/MGMS graphics prize. Journal of Molecular Graphics and Modelling, 2010, 29, 1.	2.4	0

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163	Simulation of Two Dimensional Ultraviolet (2DUV) Spectroscopy of Amyloid Fibrils. Nature Precedings, 2010, , .	0.1	0
164	Local and Global Dynamics: general discussion. Faraday Discussions, 2015, 177, 381-403.	3.2	0
165	Simulating Biomolecules: Festschrift to commemorate the 60th birthday of Charles L. Brooks III. Journal of Computational Chemistry, 2017, 38, 1111-1113.	3.3	0
166	Computer Modeling of Protein Structure. , 2001, , .		0
167	Protein Circular Dichroism: Theoretical Aspects. , 2018, , 1-3.		0
168	Quantitative protein circular dichroism calculations. Special Publication - Royal Society of Chemistry, 0, , 20-30.	0.0	0
169	Daniel Douglas Eley. 1 October 1914â€”3 September 2015. Biographical Memoirs of Fellows of the Royal Society, 2022, 73, 227-249.	0.1	0