John B O Mitchell

List of Publications by Year
in descending order

113	6,119	76326	74163
papers	citations	40 h-index	75 g-index

117	117	117	6750
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Allosteric Inhibition of Acinetobacter baumannii ATP Phosphoribosyltransferase by Protein:Dipeptide and Protein:Protein Interactions. ACS Infectious Diseases, 2022, 8, 197-209.	3.8	4
2	Degree correlations in graphs with clique clustering. Physical Review E, 2022, 105, 044314.	2.1	2
3	A Bayesian network structure learning approach to identify genes associated with stress in spleens of chickens. Scientific Reports, 2022, 12, 7482.	3.3	0
4	Random graphs with arbitrary clustering and their applications. Physical Review E, 2021, 103, 012309.	2.1	14
5	Cooperative coinfection dynamics on clustered networks. Physical Review E, 2021, 103, 042307.	2.1	3
6	Toward Physics-Based Solubility Computation for Pharmaceuticals to Rival Informatics. Journal of Chemical Theory and Computation, 2021, 17, 3700-3709.	5.3	15
7	Two-pathogen model with competition on clustered networks. Physical Review E, 2021, 103, 062308.	2.1	7
8	Exact formula for bond percolation on cliques. Physical Review E, 2021, 104, 024304.	2.1	5
9	Symbiotic and antagonistic disease dynamics on networks using bond percolation. Physical Review E, 2021, 104, 024303.	2.1	2
10	Percolation in random graphs with higher-order clustering. Physical Review E, 2021, 103, 012313.	2.1	7
11	Three machine learning models for the 2019 Solubility Challenge. ADMET and DMPK, 2020, 8, 215-250.	2.1	7
12	3. In Silico methods to predict solubility. , 2019, , 71-112.		1
13	Rational Drug Design of Antineoplastic Agents Using 3D-QSAR, Cheminformatic, and Virtual Screening Approaches. Current Medicinal Chemistry, 2019, 26, 3874-3889.	2.4	20
14	Applications of crystal structure prediction â€“ inorganic and network structures: general discussion. Faraday Discussions, 2018, 211, 613-642.	3.2	6
15	Crystal structure evaluation: calculating relative stabilities and other criteria: general discussion. Faraday Discussions, 2018, 211, 325-381.	3.2	7
16	Applications of crystal structure prediction â€“ organic molecular structures: general discussion. Faraday Discussions, 2018, 211, 493-539.	3.2	8
17	Artificial intelligence in pharmaceutical research and development. Future Medicinal Chemistry, 2018, 10, 1529-1531.	2.3	9
18	Probing the average distribution of water in organic hydrate crystal structures with radial distribution functions (RDFs). CrystEngComm, 2017, 19, 641-652.	2.6	11

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19	Enzyme function and its evolution. Current Opinion in Structural Biology, 2017, 47, 151-156.	5.7	13
20	Can human experts predict solubility better than computers?. Journal of Cheminformatics, 2017, 9, 63.	6.1	46
21	Drug Design for CNS Diseases: Polypharmacological Profiling of Compounds Using Cheminformatic, 3D-QSAR and Virtual Screening Methodologies. Frontiers in Neuroscience, 2016, 10, 265.	2.8	62
22	A Random Forest Model for Predicting Allosteric and Functional Sites on Proteins. Molecular Informatics, 2016, 35, 125-135.	2.5	27
23	Are the Sublimation Thermodynamics of Organic Molecules Predictable?. Journal of Chemical Information and Modeling, 2016, 56, 2162-2179.	5.4	28
24	Why do Sequence Signatures Predict Enzyme Mechanism? Homology versus Chemistry. Evolutionary Bioinformatics, 2015, 11, EBO.S31482.	1.2	4
25	Enzyme mechanism prediction: a template matching problem on InterPro signature subspaces. BMC Research Notes, 2015, 8, 744.	1.4	1
26	Verifying the fully â€œLaplacianisedâ€•posterior NaÃ¯ve Bayesian approach and more. Journal of Cheminformatics, 2015, 7, 27.	6.1	5
27	A note on utilising binary features as ligand descriptors. Journal of Cheminformatics, 2015, 7, 58.	6.1	0
28	Predicting Melting Points of Organic Molecules: Applications to Aqueous Solubility Prediction Using the General Solubility Equation. Molecular Informatics, 2015, 34, 715-724.	2.5	24
29	A review of methods for the calculation of solution free energies and the modelling of systems in solution. Physical Chemistry Chemical Physics, 2015, 17, 6174-6191.	2.8	389
30	The Parzen Window method: In terms of two vectors and one matrix. Pattern Recognition Letters, 2015, 63, 30-35.	4.2	6
31	Greedy and Linear Ensembles of Machine Learning Methods Outperform Single Approaches for QSPR Regression Problems. Molecular Informatics, 2015, 34, 634-647.	2.5	10
32	Predicting targets of compounds against neurological diseases using cheminformatic methodology. Journal of Computer-Aided Molecular Design, 2015, 29, 183-198.	2.9	16
33	The Natural History of Biocatalytic Mechanisms. PLoS Computational Biology, 2014, 10, e1003642.	3.2	30
34	From sequence to enzyme mechanism using multi-label machine learning. BMC Bioinformatics, 2014, 15, 150.	2.6	17
35	Machine learning methods in chemoinformatics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 468-481.	14.6	331
36	One origin for metallo-Î²-lactamase activity, or two? An investigation assessing a diverse set of reconstructed ancestral sequences based on a sample of phylogenetic trees. Journal of Molecular Evolution, 2014, 79, 117-129.	1.8	23

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37	PFClust: an optimised implementation of a parameter-free clustering algorithm. Source Code for Biology and Medicine, 2014, 9, 5.	1.7	5
38	Uniting Cheminformatics and Chemical Theory To Predict the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules. Journal of Chemical Information and Modeling, 2014, 54, 844-856.	5.4	68
39	Is Experimental Data Quality the Limiting Factor in Predicting the Aqueous Solubility of Druglike Molecules?. Molecular Pharmaceutics, 2014, 11, 2962-2972.	4.6	91
40	Predicting the protein targets for athletic performance-enhancing substances. Journal of Cheminformatics, 2013, 5, 31.	6.1	11
41	In Silico Target Predictions: Defining a Benchmarking Data Set and Comparison of Performance of the Multiclass NaÃ¯ve Bayes and Parzen-Rosenblatt Window. Journal of Chemical Information and Modeling, 2013, 53, 1957-1966.	5.4	131
42	Full â€œLaplacianisedâ€•posterior naive Bayesian algorithm. Journal of Cheminformatics, 2013, 5, 37.	6.1	14
43	4273Ï€: Bioinformatics education on low cost ARM hardware. BMC Bioinformatics, 2013, 14, 243.	2.6	19
44	PFClust: a novel parameter free clustering algorithm. BMC Bioinformatics, 2013, 14, 213.	2.6	15
45	Enzyme Informatics. Current Topics in Medicinal Chemistry, 2012, 12, 1911-1923.	2.1	20
46	Hierarchical virtual screening for the discovery of new molecular scaffolds in antibacterial hit identification. Journal of the Royal Society Interface, 2012, 9, 3196-3207.	3.4	68
47	Is EC class predictable from reaction mechanism?. BMC Bioinformatics, 2012, 13, 60.	2.6	16
48	First-Principles Calculation of the Intrinsic Aqueous Solubility of Crystalline Druglike Molecules. Journal of Chemical Theory and Computation, 2012, 8, 3322-3337.	5.3	84
49	Predicting the mechanism of phospholipidosis. Journal of Cheminformatics, 2012, 4, 2.	6.1	49
50	Winnow based identification of potent hERG inhibitors in silico: comparative assessment on different datasets. Journal of Cheminformatics, 2012, 4, .	6.1	2
51	Classifying Molecules Using a Sparse Probabilistic Kernel Binary Classifier. Journal of Chemical Information and Modeling, 2011, 51, 1539-1544.	5.4	24
52	Comments on â€œLeave-Cluster-Out Cross-Validation Is Appropriate for Scoring Functions Derived from Diverse Protein Data Setsâ€• Significance for the Validation of Scoring Functions. Journal of Chemical Information and Modeling, 2011, 51, 1739-1741.	5.4	47
53	Characterizing the complexity of enzymes on the basis of their mechanisms and structures with a bioâ€computational analysis. FEBS Journal, 2011, 278, 3835-3845.	4.7	30
54	Development and Comparison of hERG Blocker Classifiers: Assessment on Different Datasets Yields Markedly Different Results. Molecular Informatics, 2011, 30, 443-458.	2.5	37

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55	Informatics, machine learning and computational medicinal chemistry. Future Medicinal Chemistry, 2011, 3, 451-467.	2.3	11
56	Quantitative Comparison of Catalytic Mechanisms and Overall Reactions in Convergently Evolved Enzymes: Implications for Classification of Enzyme Function. PLoS Computational Biology, 2010, 6, e1000700.	3.2	33
57	Predicting Phospholipidosis Using Machine Learning. Molecular Pharmaceutics, 2010, 7, 1708-1714.	4.6	49
58	A machine learning approach to predicting proteinâ€“ligand binding affinity with applications to molecular docking. Bioinformatics, 2010, 26, 1169-1175.	4.1	619
59	Theoretical Study of the Reaction Mechanism of Streptomyces coelicolor Type II Dehydroquinase. Journal of Chemical Theory and Computation, 2009, 5, 1284-1294.	5.3	14
60	Computational toxicology: an overview of the sources of data and of modelling methods. Expert Opinion on Drug Metabolism and Toxicology, 2009, 5, 1-14.	3.3	63
61	Understanding the Functional Roles of Amino Acid Residues in Enzyme Catalysis. Journal of Molecular Biology, 2009, 390, 560-577.	4.2	117
62	Simultaneous feature selection and parameter optimisation using an artificial ant colony: case study of melting point prediction. Chemistry Central Journal, 2008, 2, 21.	2.6	26
63	A novel hybrid ultrafast shape descriptor method for use in virtual screening. Chemistry Central Journal, 2008, 2, 3.	2.6	32
64	Toxicological relationships between proteins obtained from protein target predictions of large toxicity databases. Toxicology and Applied Pharmacology, 2008, 231, 225-234.	2.8	9
65	Why Are Some Properties More Difficult To Predict than Others? A Study of QSPR Models of Solubility, Melting Point, and Log P. Journal of Chemical Information and Modeling, 2008, 48, 220-232.	5.4	165
66	Predicting Intrinsic Aqueous Solubility by a Thermodynamic Cycle. Molecular Pharmaceutics, 2008, 5, 266-279.	4.6	104
67	Ligand-Target Prediction Using Winnow and Naive Bayesian Algorithms and the Implications of Overall Performance Statistics. Journal of Chemical Information and Modeling, 2008, 48, 2313-2325.	5.4	92
68	How To Winnow Actives from Inactives:â€‰ Introducing Molecular Orthogonal Sparse Bigrams (MOSBs) and Multiclass Winnow. Journal of Chemical Information and Modeling, 2008, 48, 306-318.	5.4	17
69	MACiE (Mechanism, Annotation and Classification in Enzymes): novel tools for searching catalytic mechanisms. Nucleic Acids Research, 2007, 35, D515-D520.	14.5	64
70	Using Reaction Mechanism to Measure Enzyme Similarity. Journal of Molecular Biology, 2007, 368, 1484-1499.	4.2	39
71	The Geometry of Interactions between Catalytic Residues and their Substrates. Journal of Molecular Biology, 2007, 369, 1140-1152.	4.2	12
72	The Chemistry of Protein Catalysis. Journal of Molecular Biology, 2007, 372, 1261-1277.	4.2	43

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73	Random Forest Models To Predict Aqueous Solubility. Journal of Chemical Information and Modeling, 2007, 47, 150-158.	5.4	277
74	Scoring functions and enrichment: a case study on Hsp90. BMC Bioinformatics, 2007, 8, 27.	2.6	11
75	Support vector inductive logic programming outperforms the naive Bayes classifier and inductive logic programming for the classification of bioactive chemical compounds. Journal of Computer-Aided Molecular Design, 2007, 21, 269-280.	2.9	40
76	Chemoinformatics-Based Classification of Prohibited Substances Employed for Doping in Sport. Journal of Chemical Information and Modeling, 2006, 46, 2369-2380.	5.4	30
77	Melting Point Prediction Employing k-Nearest Neighbor Algorithms and Genetic Parameter Optimization. Journal of Chemical Information and Modeling, 2006, 46, 2412-2422.	5.4	154
78	Chemistry in bioinformatics. BMC Bioinformatics, 2005, 6, 141.	2.6	12
79	Knowledge Based Potentials: the Reverse Boltzmann Methodology, Virtual Screening and Molecular Weight Dependence. QSAR and Combinatorial Science, 2005, 24, 527-536.	1.4	10
80	Communication and re-use of chemical information in bioscience. BMC Bioinformatics, 2005, 6, 180.	2.6	15
81	MACiE: a database of enzyme reaction mechanisms. Bioinformatics, 2005, 21, 4315-4316.	4.1	47
82	A structureâ€“odour relationship study using EVA descriptors and hierarchical clustering. Organic and Biomolecular Chemistry, 2004, 2, 3250-3255.	2.8	28
83	Predicting proteinâ€“ligand binding affinities: a low scoring game?. Organic and Biomolecular Chemistry, 2004, 2, 3267-3273.	2.8	49
84	Can we predict lattice energy from molecular structure?. Acta Crystallographica Section B: Structural Science, 2003, 59, 676-685.	1.8	58
85	D-amino acid residues in peptides and proteins. Proteins: Structure, Function and Bioinformatics, 2003, 50, 563-571.	2.6	53
86	Triazinone tautomers: solid phase energetics. CrystEngComm, 2003, 5, 498.	2.6	3
87	Protein Ligand Database (PLD): additional understanding of the nature and specificity of protein-ligand complexes. Bioinformatics, 2003, 19, 1856-1857.	4.1	96
88	The Determination of the Crystal Structure of Anhydrous Theophylline by X-ray Powder Diffraction with a Systematic Search Algorithm, Lattice Energy Calculations, and13C and15N Solid-State NMR:Â A Question of Polymorphism in a Given Unit Cell. Journal of Physical Chemistry B, 2001, 105, 5818-5826.	2.6	92
89	The Relationship between the Sequence Identities of Alpha Helical Proteins in the PDB and the Molecular Similarities of Their Ligands. Journal of Chemical Information and Computer Sciences, 2001, 41, 1617-1622.	2.8	40
90	Anisotropic Repulsion Potentials for Cyanuric Chloride (C3N3Cl3) and Their Application to Modeling the Crystal Structures of Azaaromatic Chlorides. Journal of Physical Chemistry A, 2001, 105, 9961-9971.	2.5	22

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91	Evaluation of a knowledge-based potential of mean force for scoring docked protein-ligand complexes. Journal of Computational Chemistry, 2001, 22, 673-688.	3.3	22
92	A Systematic Nonempirical Method of Deriving Model Intermolecular Potentials for Organic Molecules:Â Application To Amides. Journal of Physical Chemistry A, 2000, 104, 10958-10971.	2.5	38
93	Electrostatic factors in DNA intercalation. Biopolymers, 1999, 52, 84-93.	2.4	53
94	BLEEP?potential of mean force describing protein-ligand interactions: I. Generating potential. Journal of Computational Chemistry, 1999, 20, 1165-1176.	3.3	194
95	BLEEP?potential of mean force describing protein-ligand interactions: II. Calculation of binding energies and comparison with experimental data. Journal of Computational Chemistry, 1999, 20, 1177-1185.	3.3	112
96	SATIS:â€‰ Atom Typing from Chemical Connectivity. Journal of Chemical Information and Computer Sciences, 1999, 39, 751-757.	2.8	13
97	Protein folds and functions. Structure, 1998, 6, 875-884.	3.3	207
98	Design, synthesis and structure of a zinc finger with an artificial Î²-turn. Journal of Molecular Biology, 1998, 279, 973-986.	4.2	29
99	Non-randomness in side-chain packing: the distribution of interplanar angles. , 1997, 29, 370-380.		37
100	Protein Recognition of Adenylate: An Example of a Fuzzy Recognition Template. Journal of Molecular Biology, 1996, 263, 486-500.	4.2	125
101	Multipole-based calculation of the polarization energy. Theoretica Chimica Acta, 1996, 94, 287-295.	0.8	4
102	Multiple Solution Conformations of the Integrin-Binding Cyclic Pentapeptide Cyclo(-Ser-d-Leu-Asp-Val-Pro-). Analysis of the (phi,psi) Space Available to Cyclic Pentapeptides. FEBS Journal, 1996, 242, 352-362.	0.2	31
103	Modelling the interactions of protein side-chains. Molecular Engineering, 1995, 5, 89-105.	0.2	2
104	Modelling the Interactions of Protein Side-Chains. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 119-135.	0.2	1
105	Gaussian multipoles in practice: Electrostatic energies for intermolecular potentials. Journal of Computational Chemistry, 1994, 15, 1187-1198.	3.3	77
106	Amino/Aromatic Interactions in Proteins: Is the Evidence Stacked Against Hydrogen Bonding?. Journal of Molecular Biology, 1994, 239, 315-331.	4.2	319
107	Amino/aromatic interactions. Nature, 1993, 366, 413-413.	27.8	50
108	A comparison of three theoretical approaches to the study of side-chain interactions in proteins. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 2619.	1.7	25

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109	Towards an understanding of the arginine-aspartate interaction. Journal of Molecular Biology, 1992, 226, 251-262.	4.2	103
110	On the relative strengths of amideâ€¦amide and amideâ€¦water hydrogen bonds. Chemical Physics Letters, 1991, 180, 517-523.	2.6	64
111	The nature of the N ? H?O?C hydrogen bond: An intermolecular perturbation theory study of the formamide/formaldehyde complex. Journal of Computational Chemistry, 1990, 11, 1217-1233.	3.3	104
112	On the electrostatic directionality of Nî—¸Hâ€¦Oî—»C hydrogen bonding. Chemical Physics Letters, 1989, 154, 267-272.	2.6	63
113	Diisophorone and related compounds. Part 19 Synthesis and reactions of 6,8-dibromodiisophorones. Monatshefte FÃ¼r Chemie, 1988, 119, 195-213.	1.8	7