Steven L Dixon

List of Publications by Year
in descending order

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29	4,114	279487	500791
papers	citations	23 h-index	28 g-index

31	31	31	4324
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Reliable and Accurate Solution to the Induced Fit Docking Problem for Proteinâ€“Ligand Binding. Journal of Chemical Theory and Computation, 2021, 17, 2630-2639.	2.3	60
2	AutoQSAR: an automated machine learning tool for best-practice quantitative structureâ€“activity relationship modeling. Future Medicinal Chemistry, 2016, 8, 1825-1839.	1.1	102
3	Exploring conformational search protocols for ligand-based virtual screening and 3-D QSAR modeling. Journal of Computer-Aided Molecular Design, 2015, 29, 165-182.	1.3	31
4	Kernel-Based Partial Least Squares: Application to Fingerprint-Based QSAR with Model Visualization. Journal of Chemical Information and Modeling, 2013, 53, 2312-2321.	2.5	53
5	Hole filling and library optimization: Application to commercially available fragment libraries. Bioorganic and Medicinal Chemistry, 2012, 20, 5379-5387.	1.4	16
6	Rapid Shape-Based Ligand Alignment and Virtual Screening Method Based on Atom/Feature-Pair Similarities and Volume Overlap Scoring. Journal of Chemical Information and Modeling, 2011, 51, 2455-2466.	2.5	190
7	Large-Scale Systematic Analysis of 2D Fingerprint Methods and Parameters to Improve Virtual Screening Enrichments. Journal of Chemical Information and Modeling, 2010, 50, 771-784.	2.5	301
8	Analysis and comparison of 2D fingerprints: Insights into database screening performance using eight fingerprint methods. Journal of Molecular Graphics and Modelling, 2010, 29, 157-170.	1.3	390
9	PHASE: A Novel Approach to Pharmacophore Modeling and 3D Database Searching. Chemical Biology and Drug Design, 2006, 67, 370-372.	1.5	520
10	PHASE: a new engine for pharmacophore perception, 3D QSAR model development, and 3D database screening: 1. Methodology and preliminary results. Journal of Computer-Aided Molecular Design, 2006, 20, 647-671.	1.3	963
11	Induction of Decision Trees via Evolutionary Programming. Journal of Chemical Information and Computer Sciences, 2004, 44, 862-870.	2.8	40
12	In silico models for the prediction of dose-dependent human hepatotoxicity. Journal of Computer-Aided Molecular Design, 2003, 17, 811-823.	1.3	102
13	Use of Robust Classification Techniques for the Prediction of Human Cytochrome P450 2D6 Inhibition.. ChemInform, 2003, 34, no.	0.1	0
14	Use of Robust Classification Techniques for the Prediction of Human Cytochrome P450 2D6 Inhibition. Journal of Chemical Information and Computer Sciences, 2003, 43, 1308-1315.	2.8	160
15	Quantum Mechanical Models Correlating Structure with Selectivity:â€‰Predicting the Enantioselectivity of Î²-Amino Alcohol Catalysts in Aldehyde Alkylation. Journal of the American Chemical Society, 2003, 125, 6614-6615.	6.6	100
16	Computation of the physio-chemical properties and data mining of large molecular collections. Journal of Computational Chemistry, 2002, 23, 172-183.	1.5	56
17	One-Dimensional Molecular Representations and Similarity Calculations:Â Methodology and Validation. Journal of Medicinal Chemistry, 2001, 44, 3795-3809.	2.9	90
18	Linear scaling molecular orbital calculations of biological systems using the semiempirical divide and conquer method. Journal of Computational Chemistry, 2000, 21, 1494-1504.	1.5	80

#	Article	IF	Citations
19	Investigation of classification methods for the prediction of activity in diverse chemical libraries. , 1999, 13, 533-545.		33
20	The Hidden Component of Size in Two-Dimensional Fragment Descriptors:â€‰ Side Effects on Sampling in Bioactive Libraries. Journal of Medicinal Chemistry, 1999, 42, 2887-2900.	2.9	73
21	LASSOO:Â A Generalized Directed Diversity Approach to the Design and Enrichment of Chemical Libraries. Journal of Medicinal Chemistry, 1999, 42, 4695-4704.	2.9	29
22	Parallel implementation of a divide and conquer semiempirical algorithm. Theoretical Chemistry Accounts, 1998, 99, 220-223.	0.5	14
23	Bioactive Diversity and Screening Library Selection via Affinity Fingerprinting. Journal of Chemical Information and Computer Sciences, 1998, 38, 1192-1203.	2.8	69
24	Fast, accurate semiempirical molecular orbital calculations for macromolecules. Journal of Chemical Physics, 1997, 107, 879-893.	1.2	208
25	Free Energy Perturbation Calculations Within Quantum Mechanical Methodologies. ACS Symposium Series, 1996, , 142-153.	0.5	1
26	Semiempirical molecular orbital calculations with linear system size scaling. Journal of Chemical Physics, 1996, 104, 6643-6649.	1.2	258
27	Fast geometry optimization using a modified extended HÃ¼ckel method: Results for molecules containing H, C, N, O, and F. Journal of Computational Chemistry, 1994, 15, 733-746.	1.5	17
28	Estimation of pKa for organic oxyacids using calculated atomic charges. Journal of Computational Chemistry, 1993, 14, 1460-1467.	1.5	97
29	Atomic charge calculations for quantitative structure?property relationships. Journal of Computational Chemistry, 1992, 13, 492-504.	1.5	60