

Dimitris K Agrafiotis

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

83

papers

3,111

citations

33

h-index

54

g-index

92

ext. papers

3,464

ext. citations

7.1

avg, IF

5.25

L-index

#	Paper	IF	Citations
83	Accurate prediction of clinical stroke scales and improved biomarkers of motor impairment from robotic measurements. <i>PLoS ONE</i> , 2021 , 16, e0245874	3.7	8
82	QSAR without borders. <i>Chemical Society Reviews</i> , 2020 , 49, 3525-3564	58.5	196
81	Xcellerate Investigator Portal: A New Web-Based Tool for Online Delivery of Central Laboratory Data, Reports, and Communications to Clinical Sites. <i>SLAS Technology</i> , 2020 , 25, 427-435	3	
80	A new risk and issue management system to improve productivity, quality, and compliance in clinical trials. <i>JAMIA Open</i> , 2019 , 2, 216-221	2.9	9
79	A dimensional warehouse for integrating operational data from clinical trials. <i>Database: the Journal of Biological Databases and Curation</i> , 2019 , 2019,	5	5
78	A cross-source, system-agnostic solution for clinical data review. <i>Database: the Journal of Biological Databases and Curation</i> , 2019 , 2019,	5	1
77	A late-binding, distributed, NoSQL warehouse for integrating patient data from clinical trials. <i>Database: the Journal of Biological Databases and Curation</i> , 2019 , 2019,	5	8
76	Quantifying and visualizing site performance in clinical trials. <i>Contemporary Clinical Trials Communications</i> , 2018 , 9, 108-114	1.8	4
75	Risk-based Monitoring of Clinical Trials: An Integrative Approach. <i>Clinical Therapeutics</i> , 2018 , 40, 1204-1213	3	16
74	Robotic measurement of arm movements after stroke establishes biomarkers of motor recovery. <i>Stroke</i> , 2014 , 45, 200-4	6.7	103
73	Stochastic Proximity Embedding: A Simple, Fast and Scalable Algorithm for Solving the Distance Geometry Problem 2013 , 291-311		3
72	Recognizing pitfalls in virtual screening: a critical review. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 867-81	6.1	295
71	Developing Best Practices for Descriptor-Based Property Prediction: Appropriate Matching of Datasets, Descriptors, Methods, and Expectations 2012 , 33-64		5
70	An integrated data management framework for drug discovery--from data capturing to decision support. <i>Current Topics in Medicinal Chemistry</i> , 2012 , 12, 1237-42	3	4
69	Efficient substructure searching of large chemical libraries: the ABCD chemical cartridge. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 3113-30	6.1	30
68	Power keys: a novel class of topological descriptors based on exhaustive subgraph enumeration and their application in substructure searching. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2843-51	6.1	10
67	Library enhancement through the wisdom of crowds. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 3275-86	6.1	31

66	Stochastic proximity embedding on graphics processing units: taking multidimensional scaling to a new scale. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 2852-9	6.1	2
65	Single R-Group Polymorphisms (SRPs) and R-cliffs: an intuitive framework for analyzing and visualizing activity cliffs in a single analog series. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 1122-31	6.1	24
64	Rapid communication reply to comment on: Fast determination of the optimal rotational matrix for macromolecular superpositions. <i>Journal of Computational Chemistry</i> , 2011 , 32, 185-186	3.5	6
63	Accelerating chemical database searching using graphics processing units. <i>Journal of Chemical Information and Modeling</i> , 2011 , 51, 1807-16	6.1	11
62	The 18th European symposium on quantitative structure-activity relationships. <i>Expert Opinion on Drug Discovery</i> , 2011 , 6, 453-6	6.2	2
61	Broadening access to electronic healthcare databases. <i>Nature Reviews Drug Discovery</i> , 2010 , 9, 84	64.1	19
60	Scaffold explorer: an interactive tool for organizing and mining structure-activity data spanning multiple chemotypes. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 5002-11	8.3	38
59	Fast determination of the optimal rotational matrix for macromolecular superpositions. <i>Journal of Computational Chemistry</i> , 2010 , 31, 1561-3	3.5	78
58	Stochastic Proximity Embedding: Methods and Applications. <i>Molecular Informatics</i> , 2010 , 29, 758-70	3.8	23
57	A self-organizing algorithm for modeling protein loops. <i>PLoS Computational Biology</i> , 2009 , 5, e1000478	5	24
56	Conformational analysis of macrocycles: finding what common search methods miss. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2242-59	6.1	49
55	Conformational sampling with stochastic proximity embedding and self-organizing superimposition: establishing reasonable parameters for their practical use. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2786-800	6.1	12
54	Enhanced SAR maps: expanding the data rendering capabilities of a popular medicinal chemistry tool. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 2221-30	6.1	31
53	A self-organizing algorithm for molecular alignment and pharmacophore development. <i>Journal of Computational Chemistry</i> , 2008 , 29, 965-82	3.5	22
52	Radial clustergrams: visualizing the aggregate properties of hierarchical clusters. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 69-75	6.1	18
51	Advanced biological and chemical discovery (ABCD): centralizing discovery knowledge in an inherently decentralized world. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1999-2014	6.1	60
50	Recursive distance partitioning algorithm for common pharmacophore identification. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1619-25	6.1	15
49	Self-organizing superimposition algorithm for conformational sampling. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1234-9	3.5	17

48	On the effects of permuted input on conformational sampling of drug-like molecules: an evaluation of stochastic proximity embedding. <i>Chemical Biology and Drug Design</i> , 2007 , 70, 123-33	2.9	8
47	SAR maps: a new SAR visualization technique for medicinal chemists. <i>Journal of Medicinal Chemistry</i> , 2007 , 50, 5926-37	8.3	66
46	Recent advances in chemoinformatics. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1279-93	6.1	50
45	Conformational sampling of bioactive molecules: a comparative study. <i>Journal of Chemical Information and Modeling</i> , 2007 , 47, 1067-86	6.1	91
44	A distance geometry heuristic for expanding the range of geometries sampled during conformational search. <i>Journal of Computational Chemistry</i> , 2006 , 27, 1962-9	3.5	35
43	A cluster-based strategy for assessing the overlap between large chemical libraries and its application to a recent acquisition. <i>Journal of Chemical Information and Modeling</i> , 2006 , 46, 2651-60	6.1	32
42	A QSAR model of HERG binding using a large, diverse, and internally consistent training set. <i>Chemical Biology and Drug Design</i> , 2006 , 67, 284-96	2.9	65
41	Conformational Boosting. <i>Australian Journal of Chemistry</i> , 2006 , 59, 874	1.2	5
40	A method for quantifying and visualizing the diversity of QSAR models. <i>Journal of Molecular Graphics and Modelling</i> , 2004 , 22, 275-84	2.8	16
39	Using particle swarms for the development of QSAR models based on K-nearest neighbor and kernel regression. <i>Journal of Computer-Aided Molecular Design</i> , 2003 , 17, 255-63	4.2	36
38	Stochastic proximity embedding. <i>Journal of Computational Chemistry</i> , 2003 , 24, 1215-21	3.5	114
37	A modified update rule for stochastic proximity embedding. <i>Journal of Molecular Graphics and Modelling</i> , 2003 , 22, 133-40	2.8	16
36	Exploring the nonlinear geometry of protein homology. <i>Protein Science</i> , 2003 , 12, 1604-12	6.3	10
35	A geodesic framework for analyzing molecular similarities. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 475-84		33
34	Nearest neighbor search in general metric spaces using a tree data structure with a simple heuristic. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1933-41		13
33	Conformational sampling by self-organization. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1186-91		38
32	Combinatorial informatics in the post-genomics ERA. <i>Nature Reviews Drug Discovery</i> , 2002 , 1, 337-46	64.1	92
31	Variable selection for QSAR by artificial ant colony systems. <i>SAR and QSAR in Environmental Research</i> , 2002 , 13, 417-23	3.5	51

30	A self-organizing principle for learning nonlinear manifolds. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 15869-72	11.5	79
29	Scalable methods for the construction and analysis of virtual combinatorial libraries. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2002 , 5, 167-78	1.3	17
28	Feature selection for structure-activity correlation using binary particle swarms. <i>Journal of Medicinal Chemistry</i> , 2002 , 45, 1098-107	8.3	138
27	A fractal approach for selecting an appropriate bin size for cell-based diversity estimation. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 117-22		13
26	On the use of neural network ensembles in QSAR and QSPR. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 903-11		142
25	Retrospect and prospect of virtual screening in drug discovery. <i>Current Topics in Medicinal Chemistry</i> , 2002 , 2, 1305-20	3	38
24	Nonlinear mapping of massive data sets by fuzzy clustering and neural networks. <i>Journal of Computational Chemistry</i> , 2001 , 22, 373-386	3.5	33
23	Multidimensional scaling and visualization of large molecular similarity tables. <i>Journal of Computational Chemistry</i> , 2001 , 22, 488-500	3.5	44
22	Multidimensional scaling of combinatorial libraries without explicit enumeration. <i>Journal of Computational Chemistry</i> , 2001 , 22, 1712-1722	3.5	17
21	Combinatorial networks. <i>Journal of Molecular Graphics and Modelling</i> , 2001 , 19, 571-8, 610-3	2.8	8
20	A novel method for building regression tree models for QSAR based on artificial ant colony systems. <i>Journal of Chemical Information and Computer Sciences</i> , 2001 , 41, 176-80		61
19	A constant time algorithm for estimating the diversity of large chemical libraries. <i>Journal of Chemical Information and Computer Sciences</i> , 2001 , 41, 159-67		34
18	Design and prioritization of plates for high-throughput screening. <i>Journal of Chemical Information and Computer Sciences</i> , 2001 , 41, 798-805		7
17	Multidimensional scaling and visualization of large molecular similarity tables. <i>Journal of Computational Chemistry</i> , 2001 , 22, 488-500	3.5	35
16	Kolmogorov-Smirnov statistic and its application in library design. <i>Journal of Molecular Graphics and Modelling</i> , 2000 , 18, 368-82	2.8	41
15	The Measurement of Molecular Diversity. <i>Methods and Principles in Medicinal Chemistry</i> , 2000 , 265-300	0.4	7
14	Nonlinear mapping networks. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 1356-62		60
13	Ultrafast algorithm for designing focused combinatorial arrays. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 1030-8		25

12	Stochastic similarity selections from large combinatorial libraries. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 460-70		25
11	An Efficient Implementation of Distance-Based Diversity Measures Based on α -Trees. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 51-58		49
10	Advances in diversity profiling and combinatorial series design. <i>Annual Reports in Combinatorial Chemistry and Molecular Diversity</i> , 1999 , 71-92		3
9	Advances in diversity profiling and combinatorial series design. <i>Molecular Diversity</i> , 1998 , 4, 1-22	3.1	50
8	Stochastic Algorithms for Maximizing Molecular Diversity. <i>Journal of Chemical Information and Computer Sciences</i> , 1997 , 37, 841-851		115
7	On the Use of Information Theory for Assessing Molecular Diversity. <i>Journal of Chemical Information and Computer Sciences</i> , 1997 , 37, 576-580		43
6	A new method for analyzing protein sequence relationships based on Sammon maps. <i>Protein Science</i> , 1997 , 6, 287-93	6.3	37
5	PRODEN: A new program for calculating integrated projected populations. <i>Journal of Computational Chemistry</i> , 1990 , 11, 1101-1110	3.5	3
4	Berry and turnstile processes in the pseudorotation of three phosphoranes. <i>Journal of the Chemical Society Chemical Communications</i> , 1990 , 201-203		14
3	A theoretical MNDO and AM1 SCF-MO study of dihydrogen transfer reactions. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1989 , 475		6
2	Dihydrogen transfer reactions. An SCF-MO study of the relative energies of the concerted and stepwise pathways. <i>Journal of the Chemical Society Chemical Communications</i> , 1987 , 902		6
1	Molecular Diversity 1640-1686		1