Dimitris K Agrafiotis

List of Publications by Citations

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	Recognizing pitfalls in virtual screening: a critical review. *Journal of Chemical Information and Modeling*, **2012**, 52, 867-81	6.1	295
82	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
81	On the use of neural network ensembles in QSAR and QSPR. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 903-11		142
80	Feature selection for structure-activity correlation using binary particle swarms. *Journal of Medicinal Chemistry*, **2002**, 45, 1098-107	8.3	138
79	Stochastic Algorithms for Maximizing Molecular Diversity. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 841-851		115
78	Stochastic proximity embedding. *Journal of Computational Chemistry*, **2003**, 24, 1215-21	3.5	114
77	Robotic measurement of arm movements after stroke establishes biomarkers of motor recovery. *Stroke*, **2014**, 45, 200-4	6.7	103
76	Combinatorial informatics in the post-genomics ERA. *Nature Reviews Drug Discovery*, **2002**, 1, 337-46	64.1	92
75	Conformational sampling of bioactive molecules: a comparative study. *Journal of Chemical Information and Modeling*, **2007**, 47, 1067-86	6.1	91
74	A self-organizing principle for learning nonlinear manifolds. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 15869-72	11.5	79
73	Fast determination of the optimal rotational matrix for macromolecular superpositions. *Journal of Computational Chemistry*, **2010**, 31, 1561-3	3.5	78
72	SAR maps: a new SAR visualization technique for medicinal chemists. *Journal of Medicinal Chemistry* , **2007**, 50, 5926-37	8.3	66
71	A QSAR model of HERG binding using a large, diverse, and internally consistent training set. *Chemical Biology and Drug Design*, **2006**, 67, 284-96	2.9	65
70	A novel method for building regression tree models for QSAR based on artificial ant colony systems. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 176-80		61
69	Advanced biological and chemical discovery (ABCD): centralizing discovery knowledge in an inherently decentralized world. *Journal of Chemical Information and Modeling*, **2007**, 47, 1999-2014	6.1	60
68	Nonlinear mapping networks. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1356-62		60
67	Variable selection for QSAR by artificial ant colony systems. *SAR and QSAR in Environmental Research*, **2002**, 13, 417-23	3.5	51

66	Advances in diversity profiling and combinatorial series design. *Molecular Diversity*, **1998**, 4, 1-22	3.1	50
65	Recent advances in chemoinformatics. *Journal of Chemical Information and Modeling*, **2007**, 47, 1279-93	6.1	50
64	Conformational analysis of macrocycles: finding what common search methods miss. *Journal of Chemical Information and Modeling*, **2009**, 49, 2242-59	6.1	49
63	An Efficient Implementation of Distance-Based Diversity Measures Based onk-Trees. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 51-58		49
62	Multidimensional scaling and visualization of large molecular similarity tables. *Journal of Computational Chemistry*, **2001**, 22, 488-500	3.5	44
61	On the Use of Information Theory for Assessing Molecular Diversity. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 576-580		43
60	Kolmogorov-Smirnov statistic and its application in library design. *Journal of Molecular Graphics and Modelling*, **2000**, 18, 368-82	2.8	41
59	Scaffold explorer: an interactive tool for organizing and mining structure-activity data spanning multiple chemotypes. *Journal of Medicinal Chemistry*, **2010**, 53, 5002-11	8.3	38
58	Conformational sampling by self-organization. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1186-91		38
57	Retrospect and prospect of virtual screening in drug discovery. *Current Topics in Medicinal Chemistry*, **2002**, 2, 1305-20	3	38
56	A new method for analyzing protein sequence relationships based on Sammon maps. *Protein Science*, **1997**, 6, 287-93	6.3	37
55	Using particle swarms for the development of QSAR models based on K-nearest neighbor and kernel regression. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 255-63	4.2	36
54	A distance geometry heuristic for expanding the range of geometries sampled during conformational search. *Journal of Computational Chemistry*, **2006**, 27, 1962-9	3.5	35
53	Multidimensional scaling and visualization of large molecular similarity tables. *Journal of Computational Chemistry*, **2001**, 22, 488-500	3.5	35
52	A constant time algorithm for estimating the diversity of large chemical libraries. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 159-67		34
51	A geodesic framework for analyzing molecular similarities. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 475-84		33
50	Nonlinear mapping of massive data sets by fuzzy clustering and neural networks. *Journal of Computational Chemistry*, **2001**, 22, 373-386	3.5	33
49	A cluster-based strategy for assessing the overlap between large chemical libraries and its application to a recent acquisition. *Journal of Chemical Information and Modeling*, **2006**, 46, 2651-60	6.1	32

48	Library enhancement through the wisdom of crowds. *Journal of Chemical Information and Modeling*, **2011**, 51, 3275-86	6.1	31
47	Enhanced SAR maps: expanding the data rendering capabilities of a popular medicinal chemistry tool. *Journal of Chemical Information and Modeling*, **2009**, 49, 2221-30	6.1	31
46	Efficient substructure searching of large chemical libraries: the ABCD chemical cartridge. *Journal of Chemical Information and Modeling*, **2011**, 51, 3113-30	6.1	30
45	Ultrafast algorithm for designing focused combinational arrays. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1030-8		25
44	Stochastic similarity selections from large combinatorial libraries. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 460-70		25
43	Single R-Group Polymorphisms (SRPs) and R-cliffs: an intuitive framework for analyzing and visualizing activity cliffs in a single analog series. *Journal of Chemical Information and Modeling*, **2011**, 51, 1122-31	6.1	24
42	A self-organizing algorithm for modeling protein loops. *PLoS Computational Biology*, **2009**, 5, e1000478	5	24
41	Stochastic Proximity Embedding: Methods and Applications. *Molecular Informatics*, **2010**, 29, 758-70	3.8	23
40	A self-organizing algorithm for molecular alignment and pharmacophore development. *Journal of Computational Chemistry*, **2008**, 29, 965-82	3.5	22
39	Broadening access to electronic healthcare databases. *Nature Reviews Drug Discovery*, **2010**, 9, 84	64.1	19
38	Radial clustergrams: visualizing the aggregate properties of hierarchical clusters. *Journal of Chemical Information and Modeling*, **2007**, 47, 69-75	6.1	18
37	Self-organizing superimposition algorithm for conformational sampling. *Journal of Computational Chemistry*, **2007**, 28, 1234-9	3.5	17
36	Multidimensional scaling of combinatorial libraries without explicit enumeration. *Journal of Computational Chemistry*, **2001**, 22, 1712-1722	3.5	17
35	Scalable methods for the construction and analysis of virtual combinatorial libraries. *Combinatorial Chemistry and High Throughput Screening*, **2002**, 5, 167-78	1.3	17
34	Risk-based Monitoring of Clinical Trials: An Integrative Approach. *Clinical Therapeutics*, **2018**, 40, 1204-1212	3.3	16
33	A method for quantifying and visualizing the diversity of QSAR models. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 275-84	2.8	16
32	A modified update rule for stochastic proximity embedding. *Journal of Molecular Graphics and Modelling*, **2003**, 22, 133-40	2.8	16
31	Recursive distance partitioning algorithm for common pharmacophore identification. *Journal of Chemical Information and Modeling*, **2007**, 47, 1619-25	6.1	15

30	Berry and turnstyle processes in the pseudorotation of three phosphoranes. *Journal of the Chemical Society Chemical Communications*, **1990**, 201-203		14
29	Nearest neighbor search in general metric spaces using a tree data structure with a simple heuristic. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1933-41		13
28	A fractal approach for selecting an appropriate bin size for cell-based diversity estimation. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 117-22		13
27	Conformational sampling with stochastic proximity embedding and self-organizing superimposition: establishing reasonable parameters for their practical use. *Journal of Chemical Information and Modeling*, **2009**, 49, 2786-800	6.1	12
26	Accelerating chemical database searching using graphics processing units. *Journal of Chemical Information and Modeling*, **2011**, 51, 1807-16	6.1	11
25	Power keys: a novel class of topological descriptors based on exhaustive subgraph enumeration and their application in substructure searching. *Journal of Chemical Information and Modeling*, **2011**, 51, 2843-51	6.1	10
24	Exploring the nonlinear geometry of protein homology. *Protein Science*, **2003**, 12, 1604-12	6.3	10
23	A new risk and issue management system to improve productivity, quality, and compliance in clinical trials. *JAMIA Open*, **2019**, 2, 216-221	2.9	9
22	A late-binding, distributed, NoSQL warehouse for integrating patient data from clinical trials. *Database: the Journal of Biological Databases and Curation*, **2019**, 2019,	5	8
21	On the effects of permuted input on conformational sampling of drug-like molecules: an evaluation of stochastic proximity embedding. *Chemical Biology and Drug Design*, **2007**, 70, 123-33	2.9	8
20	Combinatorial networks. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 571-8, 610-3	2.8	8
19	Accurate prediction of clinical stroke scales and improved biomarkers of motor impairment from robotic measurements. *PLoS ONE*, **2021**, 16, e0245874	3.7	8
18	The Measurement of Molecular Diversity. *Methods and Principles in Medicinal Chemistry*, **2000**, 265-300	0.4	7
17	Design and prioritization of plates for high-throughput screening. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 798-805		7
16	Rapid communication reply to comment on: Fast determination of the optimal rotational matrix for macromolecular superpositions *Journal of Computational Chemistry*, **2011**, 32, 185-186	3.5	6
15	A theoretical MNDO and AM1 SCF-MO study of dihydrogen transfer reactions. *Journal of the Chemical Society Perkin Transactions II*, **1989**, 475		6
14	Dihydrogen transfer reactions. An SCF-MO study of the relative energies of the concerted and stepwise pathways. *Journal of the Chemical Society Chemical Communications*, **1987**, 902		6
13	A dimensional warehouse for integrating operational data from clinical trials. *Database: the Journal of Biological Databases and Curation*, **2019**, 2019,	5	5

12	Developing Best Practices for Descriptor-Based Property Prediction: Appropriate Matching of Datasets, Descriptors, Methods, and Expectations **2012**, 33-64		5
11	Conformational Boosting. *Australian Journal of Chemistry*, **2006**, 59, 874	1.2	5
10	Quantifying and visualizing site performance in clinical trials. *Contemporary Clinical Trials Communications*, **2018**, 9, 108-114	1.8	4
9	An integrated data management framework for drug discovery--from data capturing to decision support. *Current Topics in Medicinal Chemistry*, **2012**, 12, 1237-42	3	4
8	Stochastic Proximity Embedding: A Simple, Fast and Scalable Algorithm for Solving the Distance Geometry Problem **2013**, 291-311		3
7	PRODEN: A new program for calculating integrated projected populations. *Journal of Computational Chemistry*, **1990**, 11, 1101-1110	3.5	3
6	Advances in diversity profiling and combinatorial series design. *Annual Reports in Combinatorial Chemistry and Molecular Diversity*, **1999**, 71-92		3
5	Stochastic proximity embedding on graphics processing units: taking multidimensional scaling to a new scale. *Journal of Chemical Information and Modeling*, **2011**, 51, 2852-9	6.1	2
4	The 18th European symposium on quantitative structure-activity relationships. *Expert Opinion on Drug Discovery*, **2011**, 6, 453-6	6.2	2
3	A cross-source, system-agnostic solution for clinical data review. *Database: the Journal of Biological Databases and Curation*, **2019**, 2019,	5	1
2	Molecular Diversity1640-1686		1
1	Xcellerate Investigator Portal: A New Web-Based Tool for Online Delivery of Central Laboratory Data, Reports, and Communications to Clinical Sites. *SLAS Technology*, **2020**, 25, 427-435	3	