Peter Murray-Rust

List of Publications by Year in descending order

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86 papers	5,445 citations	94433 37 h-index	82547 72 g-index
89 all docs	89 docs citations	89 times ranked	5299 citing authors

#	Article	IF	Citations
1	The BioPAX community standard for pathway data sharing. Nature Biotechnology, 2010, 28, 935-942.	17.5	613
2	Angular preferences of intermolecular forces around halogen centers: preferred directions of approach of electrophiles and nucleophiles around carbon-halogen bond. Journal of the American Chemical Society, 1986, 108, 4308-4314.	13.7	512
3	The Blue Obeliskâ€"Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	5.4	366
4	Intermolecular interactions of the carbon-fluorine bond: the crystallographic environment of fluorinated carboxylic acids and related structures. Journal of the American Chemical Society, 1983, 105, 3206-3214.	13.7	311
5	Directional hydrogen bonding to sp2- and sp3-hybridized oxygen atoms and its relevance to ligand-macromolecule interactions. Journal of the American Chemical Society, 1984, 106, 1018-1025.	13.7	293
6	Geometrical substituent parameters for benzene derivatives: inductive and resonance effects. Tetrahedron Letters, 1979, 20, 2283-2286.	1.4	210
7	Chemical Markup, XML, and the Worldwide Web. 1. Basic Principles. Journal of Chemical Information and Computer Sciences, 1999, 39, 928-942.	2.8	196
8	Computer retrieval and analysis of molecular geometry. 4. Intermolecular interactions. Journal of the American Chemical Society, 1979, 101, 4374-4376.	13.7	157
9	OSCAR4: a flexible architecture for chemical text-mining. Journal of Cheminformatics, 2011, 3, 41.	6.1	145
10	Chemical Name to Structure: OPSIN, an Open Source Solution. Journal of Chemical Information and Modeling, 2011, 51, 739-753.	5.4	138
11	ChemicalTagger: A tool for semantic text-mining in chemistry. Journal of Cheminformatics, 2011, 3, 17.	6.1	117
12	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	2.6	111
13	Molecular geometry of substituted benzene derivatives. IV. Analysis of variance in monosubstituted benzene rings. Acta Crystallographica Section B: Structural Science, 1983, 39, 457-468.	1.8	99
14	Chemical reaction paths. V. SN1 reaction of tetrahedral molecules. Journal of the American Chemical Society, 1975, 97, 921-922.	13.7	98
15	Chemical Markup, XML, and the World Wide Web. 4. CML Schema. Journal of Chemical Information and Computer Sciences, 2003, 43, 757-772.	2.8	95
16	Open Data in Science. Serials Review, 2008, 34, 52-64.	0.9	83
17	Conformational variability of corrins. Some methods of analysis. Journal of the American Chemical Society, 1987, 109, 3207-3215.	13.7	81
18	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	46.4	80

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19	Enhancement of the chemical semantic web through the use of InChI identifiers. Organic and Biomolecular Chemistry, 2005, 3, 1832.	2.8	78
20	Development of chemical markup language (CML) as a system for handling complex chemical content. New Journal of Chemistry, 2001, 25, 618-634.	2.8	69
21	MACiE (Mechanism, Annotation and Classification in Enzymes): novel tools for searching catalytic mechanisms. Nucleic Acids Research, 2007, 35, D515-D520.	14.5	64
22	Chemical Markup, XML and the World-Wide Web. 2. Information Objects and the CMLDOM. Journal of Chemical Information and Computer Sciences, 2001, 41, 1113-1123.	2.8	63
23	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	6.1	63
24	Iodineâ‹¯X(O, N, S) intermolecular contacts: models of thyroid hormoneî—¸protein binding interactions using information from the cambridge crystallographic data files. Journal of Molecular Structure, 1984, 112, 189-199.	3.6	62
25	High-Throughput Identification of Chemistry in Life Science Texts. Lecture Notes in Computer Science, 2006, , 107-118.	1.3	55
26	Chemical Markup, XML, and the World Wide Web. 6. CMLReact, an XML Vocabulary for Chemical Reactions. Journal of Chemical Information and Modeling, 2006, 46, 145-157.	5.4	51
27	SPECTRa: The Deposition and Validation of Primary Chemistry Research Data in Digital Repositories. Journal of Chemical Information and Modeling, 2008, 48, 1571-1581.	5.4	50
28	MACiE: a database of enzyme reaction mechanisms. Bioinformatics, 2005, 21, 4315-4316.	4.1	47
29	Chemistry for everyone. Nature, 2008, 451, 648-651.	27.8	47
30	The Quixote project: Collaborative and Open Quantum Chemistry data management in the Internet age. Journal of Cheminformatics, 2011, 3, 38.	6.1	45
31	Nuclear magnetic resonance studies of the snake toxin echistatin. 1H resonance assignments and secondary structure. FEBS Journal, 1991, 202, 323-328.	0.2	44
32	The structure and physiological activity of bonellin - a unique chlorin derived from Bonellia viridis. Pure and Applied Chemistry, 1979, 51, 1847-1864.	1.9	43
33	The solution structure of echistatin: evidence for disulphide bond rearrangement in homologous snake toxins. Protein Engineering, Design and Selection, 1992, 5, 473-477.	2.1	42
34	Representation and use of chemistry in the global electronic age. Organic and Biomolecular Chemistry, 2004, 2, 3192.	2.8	42
35	Open Data in Science. Serials Review, 2008, 34, 52-64.	0.9	42
36	Chemical Markup, XML, and the World-Wide Web. 3. Toward a Signed Semantic Chemical Web of Trust. Journal of Chemical Information and Computer Sciences, 2001, 41, 1124-1130.	2.8	40

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37	Chemical Markup, XML, and the World Wide Web. 5. Applications of Chemical Metadata in RSS Aggregators. Journal of Chemical Information and Computer Sciences, 2004, 44, 462-469.	2.8	38
38	CML: Evolution and design. Journal of Cheminformatics, 2011, 3, 44.	6.1	36
39	Computer analysis of molecular geometry. Journal of Molecular Graphics, 1985, 3, 50-59.	1.1	35
40	The Application of Chemical Multipurpose Internet Mail Extensions (Chemical MIME) Internet Standards to Electronic Mail and World Wide Web Information Exchange. Journal of Chemical Information and Computer Sciences, 1998, 38, 976-982.	2.8	33
41	A series of penicillin-derived C2-symmetric inhibitors of HIV-1 proteinase: structural and modeling studies. Journal of Medicinal Chemistry, 1993, 36, 3113-3119.	6.4	32
42	The semantics of Chemical Markup Language (CML): dictionaries and conventions. Journal of Cheminformatics, 2011, 3, 43.	6.1	31
43	Analysis of the atomic environment of quaternary ammonium groups in crystal structures, using computerized data retrieval and interactive graphics: modeling acetylcholine-receptor interactions. Journal of the American Chemical Society, 1982, 104, 5427-5430.	13.7	30
44	Hyperactive molecules and the World-Wide-Web information system. Journal of the Chemical Society Perkin Transactions II, 1995, , 7.	0.9	28
45	1,2-oxazine chemistryâ€"II. Tetrahedron, 1974, 30, 1087-1096.	1.9	25
46	Chemical Markup, XML, and the World Wide Web. 7. CMLSpect, an XML Vocabulary for Spectral Data. Journal of Chemical Information and Modeling, 2007, 47, 2015-2034.	5.4	25
47	Chemical Markup, XML and the World-Wide Web. 8. Polymer Markup Language. Journal of Chemical Information and Modeling, 2008, 48, 2118-2128.	5.4	25
48	Open Data in Science. Nature Precedings, 0, , .	0.1	25
49	Mining chemical information from open patents. Journal of Cheminformatics, 2011, 3, 40.	6.1	24
50	The semantics of Chemical Markup Language (CML) for computational chemistry : CompChem. Journal of Cheminformatics, 2012, 4, 15.	6.1	24
51	Experimental data checker: better information for organic chemists. Organic and Biomolecular Chemistry, 2004, 2, 3067.	2.8	23
52	The World-Wide Web as a chemical information tool. Chemical Society Reviews, 1997, 26, 1.	38.1	22
53	Chemical documents: machine understanding and automated information extraction. Organic and Biomolecular Chemistry, 2004, 2, 3294.	2.8	21
54	Engineering Polymer Informatics: Towards the Computerâ€Aided Design of Polymers. Macromolecular Rapid Communications, 2008, 29, 615-632.	3.9	21

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55	Scientific publications in XML - towards a global knowledge base. Data Science Journal, 2002, 1, 84-98.	1.3	20
56	The structures of anhydrobonellin and bonellin, the physiologically active pigment from the marine echiuroid. Tetrahedron Letters, 1978, 19, 1881-1884.	1.4	19
57	Using Workflows to Explore and Optimise Named Entity Recognition for Chemistry. PLoS ONE, 2011, 6, e20181.	2.5	18
58	Mapping the atomic environment of functional groups: turning 3D scatter plots into pseudo-density contours. Journal of Molecular Graphics, 1984, 2, 43-46.	1.1	17
59	STMML. A markup language for scientific, technical and medical publishing. Data Science Journal, 2002, 1, 128-192.	1.3	17
60	A global resource for computational chemistry. Journal of Molecular Modeling, 2005, 11, 532-541.	1.8	16
61	The Stability and Conformation of the 1,3,6,8-Tetraazatricyclo[4.4.1.13,8]dodecane System: the Structure of the Condensation Product of 1,2-Diaminocyclohexane and Formaldehyde. Canadian Journal of Chemistry, 1975, 53, 1933-1935.	1.1	15
62	The geometry of the thioester group and its implications for the chemistry of acyl coenzyme a. Archives of Biochemistry and Biophysics, 1983, 222, 22-34.	3.0	15
63	Communication and re-use of chemical information in bioscience. BMC Bioinformatics, 2005, 6, 180.	2.6	15
64	Chemistry in bioinformatics. BMC Bioinformatics, 2005, 6, 141.	2.6	12
65	A new publishing paradigm: STM articles as part of the semantic web. Learned Publishing, 2001, 14, 177-182.	1.7	11
66	CMLLite: a design philosophy for CML. Journal of Cheminformatics, 2011, 3, 39.	6.1	11
67	Computer analysis of molecular geometry, part VII: the identification of chemical fragments in the cambridge structural data file. Journal of Molecular Graphics, 1985, 3, 60-68.	1.1	9
68	CML tools and information flow in atomic scale simulations. Molecular Simulation, 2005, 31, 315-322.	2.0	9
69	Molecular dynamics in a grid computing environment: experiences using DL_POLY_3 within theeMinerals escience project. Molecular Simulation, 2006, 32, 945-952.	2.0	9
70	Changing computational research. The challenges ahead. Source Code for Biology and Medicine, 2012, 7, 2.	1.7	8
71	Standards-based curation of a decade-old digital repository dataset of molecular information. Journal of Cheminformatics, 2015, 7, 43.	6.1	8
72	SPECTRa-T: Machine-Based Data Extraction and Semantic Searching of Chemistry e-Theses. Journal of Chemical Information and Modeling, 2010, 50, 251-261.	5.4	7

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73	First-Principles Thermochemistry for Gas Phase Species in an Industrial Rutile Chlorinator. Journal of Physical Chemistry A, 2010, 114, 11825-11832.	2.5	7
74	The semantic architecture of the World-Wide Molecular Matrix (WWMM). Journal of Cheminformatics, 2011, 3, 42.	6.1	7
75	Open Bibliography for Science, Technology, and Medicine. Journal of Cheminformatics, 2011, 3, 47.	6.1	6
76	Ami - The chemist's amanuensis. Journal of Cheminformatics, 2011, 3, 45.	6.1	5
77	Semantic science and its communication - a personal view. Journal of Cheminformatics, 2011, 3, 48.	6.1	5
78	CIFXML: a schema and toolkit for managing CIFs in XML. Journal of Applied Crystallography, 2011, 44, 628-634.	4.5	5
79	Semantic physical science. Journal of Cheminformatics, 2012, 4, 14.	6.1	3
80	An eâ€Science data infrastructure for simulations within Grid computing environment: methods, approaches and practice. Concurrency Computation Practice and Experience, 2013, 25, 385-409.	2.2	3
81	CHIC - Converting Hamburgers into Cows. , 2009, , .		2
82	pygetpapers: a Python library for automated retrieval of scientific literature. Journal of Open Source Software, 2022, 7, 4451.	4.6	2
83	Computational Grids for Mid-Sized Collaborative Projects: The eMinerals Experience. , 2006, , .		1
84	Open Chemistry. Nature Precedings, 2007, , .	0.1	0
85	Shouldn't enantiomeric purity be included in the 'minimum information about a bioactive entity? Response from the MIABE group. Nature Reviews Drug Discovery, 2012, 11, 730-730.	46.4	0
86	The PIMMS Project and Natural Language Processing for Climate Science. , 2016, , 247-269.		0