Christoph C Steinbeck

List of Publications by Year
in descending order

152	11,228	36203	33814
papers	citations	51 h-index	99 g-index

188	188	188	14938
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The Chemistry Development Kit (CDK):â€‰ An Open-Source Java Library for Chemo- and Bioinformatics. Journal of Chemical Information and Computer Sciences, 2003, 43, 493-500.	2.8	904
2	ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. Journal of Cheminformatics, 2016, 8, 61.	2.8	779
3	ChEBI in 2016: Improved services and an expanding collection of metabolites. Nucleic Acids Research, 2016, 44, D1214-D1219.	6.5	752
4	MetaboLightsâ€”an open-access general-purpose repository for metabolomics studies and associated meta-data. Nucleic Acids Research, 2013, 41, D781-D786.	6.5	578
5	The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. Nucleic Acids Research, 2012, 41, D456-D463.	6.5	508
6	Recent Developments of the Chemistry Development Kit (CDK) - An Open-Source Java Library for Chemo- and Bioinformatics. Current Pharmaceutical Design, 2006, 12, 2111-2120.	0.9	418
7	The Blue Obeliskâ€”Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	2.5	366
8	Toward interoperable bioscience data. Nature Genetics, 2012, 44, 121-126.	9.4	362
9	The role of reporting standards for metabolite annotation and identification in metabolomic studies. GigaScience, 2013, 2, 13.	3.3	333
10	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	2.8	275
11	Chemical Entities of Biological Interest: an update. Nucleic Acids Research, 2010, 38, D249-D254.	6.5	248
12	Review on natural products databases: where to find data in 2020. Journal of Cheminformatics, 2020, 12, 20.	2.8	243
13	COCONUT online: Collection of Open Natural Products database. Journal of Cheminformatics, 2021, 13, 2.	2.8	223
14	Navigating freely-available software tools for metabolomics analysis. Metabolomics, 2017, 13, 106.	1.4	173
15	Discovering and linking public omics data sets using the Omics Discovery Index. Nature Biotechnology, 2017, 35, 406-409.	9.4	159
16	MetaboLights: An Openâ€Access Database Repository for Metabolomics Data. Current Protocols in Bioinformatics, 2016, 53, 14.13.1-14.13.18.	25.8	147
17	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	1.4	140
18	The mzTab Data Exchange Format: Communicating Mass-spectrometry-based Proteomics and Metabolomics Experimental Results to a Wider Audience. Molecular and Cellular Proteomics, 2014, 13, 2765-2775.	2.5	130

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19	NMRShiftDBConstructing a Free Chemical Information System with Open-Source Components. Journal of Chemical Information and Computer Sciences, 2003, 43, 1733-1739.	2.8	127
20	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. Journal of Proteome Research, 2016, 15, 360-373.	1.8	122
21	KNIME-CDK: Workflow-driven cheminformatics. BMC Bioinformatics, 2013, 14, 257.	1.2	119
22	NMRShiftDB â€“ compound identification and structure elucidation support through a free community-built web database. Phytochemistry, 2004, 65, 2711-2717.	1.4	113
23	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	1.2	111
24	Current Challenges in Plant Eco-Metabolomics. International Journal of Molecular Sciences, 2018, 19, 1385.	1.8	106
25	Building blocks for automated elucidation of metabolites: Machine learning methods for NMR prediction. BMC Bioinformatics, 2008, 9, 400.	1.2	97
26	Data standards can boost metabolomics research, and if there is a will, there is a way. Metabolomics, 2016, 12, 14.	1.4	97
27	Automated structure prediction of trans-acyltransferase polyketide synthase products. Nature Chemical Biology, 2019, 15, 813-821.	3.9	94
28	The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research. Natural Product Reports, 2019, 36, 35-107.	5.2	92
29	The LOTUS initiative for open knowledge management in natural products research. ELife, 0, 11, .	2.8	90
30	Recent developments in automated structure elucidation of natural products. Natural Product Reports, 2004, 21, 512.	5.2	86
31	Genome-Wide Association Study of Metabolic Traits Reveals Novel Gene-Metabolite-Disease Links. PLoS Genetics, 2014, 10, e1004132.	1.5	86
32	The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web. PLoS ONE, 2011, 6, e25513.	1.1	86
33	Rheaâ€”a manually curated resource of biochemical reactions. Nucleic Acids Research, 2012, 40, D754-D760.	6.5	84
34	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	21.5	80
35	MetaboLights: towards a new COSMOS of metabolomics data management. Metabolomics, 2012, 8, 757-760.	1.4	79
36	Reaction Decoder Tool (RDT): extracting features from chemical reactions. Bioinformatics, 2016, 32, 2065-2066.	1.8	73

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37	JChemPaint - Using the Collaborative Forces of the Internet to Develop a Free Editor for 2D Chemical Structures. Molecules, 2000, 5, 93-98.	1.7	70
38	A decade after the metabolomics standards initiative it's time for a revision. Scientific Data, 2017, 4, 170138.	2.4	70
39	LipidHome: A Database of Theoretical Lipids Optimized for High Throughput Mass Spectrometry Lipidomics. PLoS ONE, 2013, 8, e61951.	1.1	69
40	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. Metabolomics, 2017, 13, 12.	1.4	69
41	Standards for Reporting Enzyme Data: The STRENDA Consortium: What it aims to do and why it should be helpful. Perspectives in Science, 2014, 1, 131-137.	0.6	65
42	SENECA:â€‰ A Platform-Independent, Distributed, and Parallel System for Computer-Assisted Structure Elucidation in Organic Chemistry. Journal of Chemical Information and Computer Sciences, 2001, 41, 1500-1507.	2.8	63
43	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	2.8	63
44	Natural product-likeness score revisited: an open-source, open-data implementation. BMC Bioinformatics, 2012, 13, 106.	1.2	63
45	eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics, 2015, 6, 10.	0.9	63
46	The Time Is Right to Focus on Model Organism Metabolomes. Metabolites, 2016, 6, 8.	1.3	63
47	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61
48	Compliance with minimum information guidelines in public metabolomics repositories. Scientific Data, 2017, 4, 170137.	2.4	61
49	NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. Magnetic Resonance in Chemistry, 2018, 56, 703-715.	1.1	61
50	PhenoMeNal: processing and analysis of metabolomics data in the cloud. GigaScience, 2019, 8, .	3.3	60
51	CDK-Taverna: an open workflow environment for cheminformatics. BMC Bioinformatics, 2010, 11, 159.	1.2	54
52	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	1.2	52
53	Bioinformatics Meets User-Centred Design: A Perspective. PLoS Computational Biology, 2012, 8, e1002554.	1.5	50
54	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. Analytical Chemistry, 2018, 90, 649-656.	3.2	50

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55	The MetaboLights repository: curation challenges in metabolomics. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat029.	1.4	46
56	Metabolomics: The Stethoscope for the Twenty-First Century. Medical Principles and Practice, 2021, 30, 301-310.	1.1	46
57	Dovetailing biology and chemistry: integrating the Gene Ontology with the ChEBI chemical ontology. BMC Genomics, 2013, 14, 513.	1.2	45
58	Alkaloids from Dactylicapnos torulosa. Phytochemistry, 1995, 40, 299-305.	1.4	44
59	Updates in Rheaâ€"a manually curated resource of biochemical reactions. Nucleic Acids Research, 2015, 43, D459-D464.	6.5	41
60	DECIMER: towards deep learning for chemical image recognition. Journal of Cheminformatics, 2020, 12, 65.	2.8	41
61	Structure-based classification and ontology in chemistry. Journal of Cheminformatics, 2012, 4, 8.	2.8	40
62	Spectrometrically monitored selection experiments: quantitative laser desorption mass spectrometry of small chemical libraries. Chemistry and Biology, 1997, 4, 63-77.	6.2	39
63	Global open data management in metabolomics. Current Opinion in Chemical Biology, 2017, 36, 58-63.	2.8	39
64	Synthesis of Carba-Porphyrinoids from Tripyrranes and Unsaturated Dialdehydes. Synthesis, 1996, 1996, 336-340.	1.2	35
65	BiNChE: A web tool and library for chemical enrichment analysis based on the ChEBI ontology. BMC Bioinformatics, 2015, 16, 56.	1.2	35
66	A review of optical chemical structure recognition tools. Journal of Cheminformatics, 2020, 12, 60.	2.8	35
67	Further isoflavonoid metabolites from Millettia griffoniana (Bail). Phytochemistry, 2001, 56, 363-368.	1.4	31
68	Performance Validation of Neural Network Based ¹³C NMR Prediction Using a Publicly Available Data Source. Journal of Chemical Information and Modeling, 2008, 48, 550-555.	2.5	29
69	DECIMER 1.0: deep learning for chemical image recognition using transformers. Journal of Cheminformatics, 2021, 13, 61.	2.8	29
70	Geminal Bismethylation Prevents Polyketide Oxidation and Dimerization in the Benastatin Pathway. Angewandte Chemie - International Edition, 2007, 46, 7035-7038.	7.2	28
71	Dissemination of metabolomics results: role of MetaboLights and COSMOS. GigaScience, 2013, 2, 8.	3.3	28
72	NaPLeS: a natural products likeness scorerâ€"web application and database. Journal of Cheminformatics, 2019, 11, 55.	2.8	28

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73	LUCYâ€”A Program for Structure Elucidation from NMR Correlation Experiments. Angewandte Chemie International Edition in English, 1996, 35, 1984-1986.	4.4	26
74	The Role of Ionic Backbones in RNA Structure:Â An Unusually Stable Non-Watsonâ“Crick Duplex of a Nonionic Analog in an Apolar Medium. Journal of the American Chemical Society, 1998, 120, 11576-11580.	6.6	26
75	A Database for Chemical Proteomics: ChEBI. Methods in Molecular Biology, 2012, 803, 273-296.	0.4	26
76	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.	2.5	25
77	Efficient ring perception for the Chemistry Development Kit. Journal of Cheminformatics, 2014, 6, 3.	2.8	25
78	STOUT: SMILES to IUPAC names using neural machine translation. Journal of Cheminformatics, 2021, 13, 34.	2.8	25
79	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. Research Ideas and Outcomes, 0, 6, .	1.0	25
80	New developments on the cheminformatics open workflow environment CDK-Taverna. Journal of Cheminformatics, 2011, 3, 54.	2.8	23
81	ChEBI: a chemistry ontology and database. Journal of Cheminformatics, 2010, 2, .	2.8	22
82	A large-scale protein-function database. Nature Chemical Biology, 2010, 6, 785-785.	3.9	22
83	Interoperable and scalable data analysis with microservices: applications in metabolomics. Bioinformatics, 2019, 35, 3752-3760.	1.8	22
84	Identification of Two Chromenes fromCalea serrataby Semiautomatic Structure Elucidation. Journal of Natural Products, 1997, 60, 627-628.	1.5	21
85	Classification and comparison of ligand-binding sites derived from grid-mapped knowledge-based potentials. Journal of Molecular Graphics and Modelling, 2006, 24, 328-340.	1.3	21
86	Evolutionary-Algorithm-Based Strategy for Computer-Assisted Structure Elucidation. Journal of Chemical Information and Computer Sciences, 2004, 44, 489-498.	2.8	20
87	Self-organizing ontology of biochemically relevant small molecules. BMC Bioinformatics, 2012, 13, 3.	1.2	20
88	Building blocks for automated elucidation of metabolites: natural product-likeness for candidate ranking. BMC Bioinformatics, 2014, 15, 234.	1.2	20
89	Solution Structure of the Aminoacyl-Capped Oligodeoxyribonucleotide Duplex (W-TGCGCAC)2â€. Biochemistry, 1999, 38, 12597-12606.	1.2	19
90	So what have data standards ever done for us? The view from metabolomics. Genome Medicine, 2010, 2, 38.	3.6	19

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91	The EBI enzyme portal. Nucleic Acids Research, 2013, 41, D773-D780.	6.5	19
92	libChEBI: an API for accessing the ChEBI database. Journal of Cheminformatics, 2016, 8, 11.	2.8	19
93	NFDI4Chem: Shaping a Digital and Cultural Change in Chemistry. Angewandte Chemie - International Edition, 2019, 58, 10766-10768.	7.2	19
94	Too sweet: cheminformatics for deglycosylation in natural products. Journal of Cheminformatics, 2020, 12, 67.	2.8	19
95	ISA API: An open platform for interoperable life science experimental metadata. GigaScience, 2021, 10, .	3.3	19
96	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	19
97	OrChem - An open source chemistry search engine for OracleÂ®. Journal of Cheminformatics, 2009, 1, 17.	2.8	18
98	A lost opportunity for science: journals promote data sharing in metabolomics but do not enforce it. Metabolomics, 2018, 14, 16.	1.4	17
99	A Metadata description of the data in "A metabolomic comparison of urinary changes in type 2 diabetes in mouse, rat, and human.". BMC Research Notes, 2011, 4, 272.	0.6	16
100	The Enzyme Portal: a case study in applying user-centred design methods in bioinformatics. BMC Bioinformatics, 2013, 14, 103.	1.2	16
101	MASPA Program Predicting Mass Spectra of Combinatorial Libraries. Journal of Chemical Information and Computer Sciences, 1997, 37, 449-457.	2.8	15
102	Expanding the Rubterolone Family: Intrinsic Reactivity and Directed Diversification of PKSâ€derived Pyrans. Chemistry - A European Journal, 2018, 24, 11319-11324.	1.7	15
103	Userscripts for the Life Sciences. BMC Bioinformatics, 2007, 8, 487.	1.2	14
104	In vivoandin vitroidentification ofZ-BOX C â€“ a new bilirubin oxidation end product. Organic and Biomolecular Chemistry, 2018, 16, 3553-3555.	1.5	14
105	Gene Cluster Activation in a Bacterial Symbiont Leads to Halogenated Angucyclic Maduralactomycins and Spirocyclic Actinospirols. Organic Letters, 2020, 22, 2634-2638.	2.4	14
106	MassCascade: Visual Programming for LCâ€MS Data Processing in Metabolomics. Molecular Informatics, 2014, 33, 307-310.	1.4	12
107	The Potential Utility of Predicted One Bond Carbon-Proton Coupling Constants in the Structure Elucidation of Small Organic Molecules by NMR Spectroscopy. PLoS ONE, 2014, 9, e111576.	1.1	12
108	Metabolic differences in ripening of Solanum lycopersicum â€˜Ailsa Craigâ€™ and three monogenic mutants. Scientific Data, 2014, 1, 140029.	2.4	12

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109	mzML2ISA & nmrML2ISA: generating enriched ISA-Tab metadata files from metabolomics XML data. Bioinformatics, 2017, 33, 2598-2600.	1.8	12
110	A 4-methyl-7-hydroxyphthalide glycoside and other constituents from Quillaja saponaria molina. Phytochemistry, 1995, 40, 1313-1315.	1.4	11
111	Alkaloids fromThalictrum przewalskii. Planta Medica, 1998, 64, 165-171.	0.7	11
112	Ten recommendations for software engineering in research. GigaScience, 2014, 3, 31.	3.3	11
113	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	11
114	SpeckTackle: JavaScript charts for spectroscopy. Journal of Cheminformatics, 2015, 7, 17.	2.8	10
115	Surge: a fast open-source chemical graph generator. Journal of Cheminformatics, 2022, 14, 24.	2.8	10
116	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. ChemInform, 2003, 34, no.	0.1	9
117	A molecular fragment cheminformatics roadmap for mesoscopic simulation. Journal of Cheminformatics, 2014, 6, 45.	2.8	9
118	Automated assembly of species metabolomes through data submission into a public repository. GigaScience, 2017, 6, 1-4.	3.3	9
119	ErtlFunctionalGroupsFinder: automated rule-based functional group detection with the Chemistry Development Kit (CDK). Journal of Cheminformatics, 2019, 11, 37.	2.8	9
120	DECIMER-Segmentation: Automated extraction of chemical structure depictions from scientific literature. Journal of Cheminformatics, 2021, 13, 20.	2.8	8
121	OntoQuery: easy-to-use web-based OWL querying. Bioinformatics, 2013, 29, 2955-2957.	1.8	7
122	Metingear: a development environment for annotating genome-scale metabolic models. Bioinformatics, 2013, 29, 2213-2215.	1.8	7
123	NFDI4Chem: Digitalen und kulturellen Wandel in der Chemie gestalten. Angewandte Chemie, 2019, 131, 10880-10882.	1.6	7
124	MAYGEN: an open-source chemical structure generator for constitutional isomers based on the orderly generation principle. Journal of Cheminformatics, 2021, 13, 48.	2.8	7
125	DECIMERâ€"hand-drawn molecule images dataset. Journal of Cheminformatics, 2022, 14, .	2.8	7
126	In support of the BMRB. Nature Structural and Molecular Biology, 2012, 19, 854-860.	3.6	6

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127	Performance of chemical structure string representations for chemical image recognition using transformers. , 2022, 1, 84-90.		6
128	From Databases to Big Data. , 2016, , 317-331.		5
129	Towards automatic classification within the ChEBI ontology. Nature Precedings, 2009, , .	0.1	4
130	Description and Analysis of Glycosidic Residues in the Largest Open Natural Products Database. Biomolecules, 2021, 11, 486.	1.8	4
131	Chemical graph generators. PLoS Computational Biology, 2021, 17, e1008504.	1.5	4
132	A Catalog of Natural Products Occurring in Watermelonâ€"Citrullus lanatus. Frontiers in Nutrition, 2021, 8, 729822.	1.6	4
133	RanDepict: Random chemical structure depiction generator. Journal of Cheminformatics, 2022, 14, .	2.8	3
134	OrChem: an open source chemistry search engine for Oracle. Journal of Cheminformatics, 2010, 2, .	2.8	2
135	Progress on an open source computer-assisted structure elucidation suite (SENECA). Journal of Cheminformatics, 2010, 2, .	2.8	2
136	Eine offene NMRâ€Datenbank. Nachrichten Aus Der Chemie, 2005, 53, 1039-1041.	0.0	1
137	Computational metabolomics â€“ a field at the boundaries of cheminformatics and bioinformatics. Journal of Cheminformatics, 2011, 3, .	2.8	1
138	Molecule Set Comparator (MSC): a CDK-based open richâ€client tool for molecule set similarity evaluations. Journal of Cheminformatics, 2021, 13, 5.	2.8	1
139	Accessing and Using Chemical Property Databases. Methods in Molecular Biology, 2012, 929, 193-219.	0.4	1
140	Draft genome assembly and sequencing dataset of the marine diatom Skeletonema cf. costatum RCC75. Data in Brief, 2022, 41, 107931.	0.5	1
141	Evolutionary-Algorithm-Based Strategy for Computer-Assisted Structure Elucidation.. ChemInform, 2004, 35, no.	0.1	0
142	Recent Developments in Automated Structure Elucidation of Natural Products. ChemInform, 2004, 35, no.	0.1	0
143	Creating chemo- & bioinformatics workflows, further developments within the CDK-Taverna Project. Chemistry Central Journal, 2008, 2, .	2.6	0
144	ChEBI â€“ an Open-access Chemistry Resource for the Life Sciences:*Facilities for On-line Submission and Curation. Nature Precedings, 2010, , .	0.1	0

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145	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.	21.5	0
146	Structured chemical class definitions and automated matching for chemical ontology evolution. Journal of Cheminformatics, 2012, 4, .	2.8	0
147	Expanding natural product chemistry resources at the EBI. Journal of Cheminformatics, 2013, 5, .	2.8	0
148	Ontologies in Chemoinformatics. , 2017, , 2163-2181.		0
149	Frontispiece: Expanding the Rubterolone Family: Intrinsic Reactivity and Directed Diversification of PKS-derived Pyrans. Chemistry - A European Journal, 2018, 24, .	1.7	0
150	Meet the Editors-in-Chief. Analytical Science Advances, 2020, 1, 4.	1.2	0
151	Ontologies in Cheminformatics. , 2016, , 1-19.		0
152	Notes on the Treatment of Charged Particles for Studying Cyclotide/Membrane Interactions with Dissipative Particle Dynamics. Membranes, 2022, 12, 619.	1.4	0