Christoph C Steinbeck

List of Publications by Citations

146 papers	8,173 citations	47 h-index	88 g-index
188 ext. papers	9,972 ext. citations	8.6 avg, IF	6.07 L-index

#	Paper	IF	Citations
146	The Chemistry Development Kit (CDK): an open-source Java library for Chemo- and Bioinformatics. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 493-500		731
145	MetaboLights--an open-access general-purpose repository for metabolomics studies and associated meta-data. *Nucleic Acids Research*, **2013**, 41, D781-6	20.1	483
144	The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. *Nucleic Acids Research*, **2013**, 41, D456-63	20.1	425
143	ChEBI in 2016: Improved services and an expanding collection of metabolites. *Nucleic Acids Research*, **2016**, 44, D1214-9	20.1	399
142	Recent developments of the chemistry development kit (CDK) - an open-source java library for chemo- and bioinformatics. *Current Pharmaceutical Design*, **2006**, 12, 2111-20	3.3	373
141	The Blue Obelisk-interoperability in chemical informatics. *Journal of Chemical Information and Modeling*, **2006**, 46, 991-8	6.1	341
140	ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. *Journal of Cheminformatics*, **2016**, 8, 61	8.6	327
139	Toward interoperable bioscience data. *Nature Genetics*, **2012**, 44, 121-6	36.3	286
138	Chemical Entities of Biological Interest: an update. *Nucleic Acids Research*, **2010**, 38, D249-54	20.1	212
137	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. *Journal of Cheminformatics*, **2017**, 9, 33	8.6	167
136	Navigating freely-available software tools for metabolomics analysis. *Metabolomics*, **2017**, 13, 106	4.7	131
135	Review on natural products databases: where to find data in 2020. *Journal of Cheminformatics*, **2020**, 12, 20	8.6	121
134	MetaboLights: An Open-Access Database Repository for Metabolomics Data. *Current Protocols in Bioinformatics*, **2016**, 53, 14.13.1-14.13.18	24.2	111
133	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. *Metabolomics*, **2015**, 11, 1587-1597	4.7	109
132	Discovering and linking public omics data sets using the Omics Discovery Index. *Nature Biotechnology*, **2017**, 35, 406-409	44.5	105
131	NMRShiftDB-constructing a free chemical information system with open-source components. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1733-9		99
130	The mzTab data exchange format: communicating mass-spectrometry-based proteomics and metabolomics experimental results to a wider audience. *Molecular and Cellular Proteomics*, **2014**, 13, 2765-75	7.6	96

129	NMRShiftDB -- compound identification and structure elucidation support through a free community-built web database. *Phytochemistry*, **2004**, 65, 2711-7	4	96
128	Recommendations and Standardization of Biomarker Quantification Using NMR-Based Metabolomics with Particular Focus on Urinary Analysis. *Journal of Proteome Research*, **2016**, 15, 360-73	5.6	94
127	KNIME-CDK: Workflow-driven cheminformatics. *BMC Bioinformatics*, **2013**, 14, 257	3.6	88
126	Data standards can boost metabolomics research, and if there is a will, there is a way. *Metabolomics* , **2016**, 12, 14	4.7	85
125	Bioclipse: an open source workbench for chemo- and bioinformatics. *BMC Bioinformatics*, **2007**, 8, 59	3.6	82
124	Recent developments in automated structure elucidation of natural products. *Natural Product Reports*, **2004**, 21, 512-8	15.1	82
123	Building blocks for automated elucidation of metabolites: machine learning methods for NMR prediction. *BMC Bioinformatics*, **2008**, 9, 400	3.6	80
122	Structured chemical class definitions and automated matching for chemical ontology evolution. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
121	Expanding natural product chemistry resources at the EBI. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
120	Creating chemo- & bioinformatics workflows, further developments within the CDK-Taverna Project. *Chemistry Central Journal*, **2008**, 2,		78
119	Genome-wide association study of metabolic traits reveals novel gene-metabolite-disease links. *PLoS Genetics*, **2014**, 10, e1004132	6	70
118	Minimum information about a bioactive entity (MIABE). *Nature Reviews Drug Discovery*, **2011**, 10, 661-9	64.1	69
117	The chemical information ontology: provenance and disambiguation for chemical data on the biological semantic web. *PLoS ONE*, **2011**, 6, e25513	3.7	65
116	MetaboLights: towards a new COSMOS of metabolomics data management. *Metabolomics*, **2012**, 8, 757-760	4.7	64
115	COCONUT online: Collection of Open Natural Products database. *Journal of Cheminformatics*, **2021**, 13, 2	8.6	64
114	Current Challenges in Plant Eco-Metabolomics. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	63
113	The value of universally available raw NMR data for transparency, reproducibility, and integrity in natural product research. *Natural Product Reports*, **2019**, 36, 35-107	15.1	63
112	Rhea--a manually curated resource of biochemical reactions. *Nucleic Acids Research*, **2012**, 40, D754-60	20.1	63

111	LipidHome: a database of theoretical lipids optimized for high throughput mass spectrometry lipidomics. *PLoS ONE*, **2013**, 8, e61951	3.7	59
110	JChemPaint - Using the Collaborative Forces of the Internet to Develop a Free Editor for 2D Chemical Structures. *Molecules*, **2000**, 5, 93-98	4.8	55
109	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. *Metabolomics*, **2017**, 13, 12	4.7	52
108	SENECA: A platform-independent, distributed, and parallel system for computer-assisted structure elucidation in organic chemistry. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1500-7		51
107	Automated structure prediction of trans-acyltransferase polyketide synthase products. *Nature Chemical Biology*, **2019**, 15, 813-821	11.7	49
106	eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. *Journal of Biomedical Semantics*, **2015**, 6, 10	2.2	48
105	SPLASH, a hashed identifier for mass spectra. *Nature Biotechnology*, **2016**, 34, 1099-1101	44.5	48
104	Natural product-likeness score revisited: an open-source, open-data implementation. *BMC Bioinformatics*, **2012**, 13, 106	3.6	48
103	Reaction Decoder Tool (RDT): extracting features from chemical reactions. *Bioinformatics*, **2016**, 32, 2065-6	7.6	48
102	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	0.8	47
101	CDK-Taverna: an open workflow environment for cheminformatics. *BMC Bioinformatics*, **2010**, 11, 159	3.6	47
100	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. *Journal of Cheminformatics*, **2011**, 3, 37	8.6	46
99	Bioclipse 2: a scriptable integration platform for the life sciences. *BMC Bioinformatics*, **2009**, 10, 397	3.6	46
98	A decade after the metabolomics standards initiative it's time for a revision. *Scientific Data*, **2017**, 4, 170138	8.2	45
97	NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. *Magnetic Resonance in Chemistry*, **2018**, 56, 703-715	2.1	43
96	Compliance with minimum information guidelines in public metabolomics repositories. *Scientific Data*, **2017**, 4, 170137	8.2	43
95	The Time Is Right to Focus on Model Organism Metabolomes. *Metabolites*, **2016**, 6,	5.6	43
94	Bioinformatics meets user-centred design: a perspective. *PLoS Computational Biology*, **2012**, 8, e1002554	5	42

93	PhenoMeNal: processing and analysis of metabolomics data in the cloud. *GigaScience*, **2019**, 8,	7.6	41
92	The MetaboLights repository: curation challenges in metabolomics. *Database: the Journal of Biological Databases and Curation*, **2013**, 2013, bat029	5	40
91	nmrML: A Community Supported Open Data Standard for the Description, Storage, and Exchange of NMR Data. *Analytical Chemistry*, **2018**, 90, 649-656	7.8	37
90	Updates in Rhea--a manually curated resource of biochemical reactions. *Nucleic Acids Research*, **2015**, 43, D459-64	20.1	37
89	Dovetailing biology and chemistry: integrating the Gene Ontology with the ChEBI chemical ontology. *BMC Genomics*, **2013**, 14, 513	4.5	35
88	Spectrometrically monitored selection experiments: quantitative laser desorption mass spectrometry of small chemical libraries. *Chemistry and Biology*, **1997**, 4, 63-77		35
87	Alkaloids from Dactylicapnos torulosa. *Phytochemistry*, **1995**, 40, 299-305	4	32
86	Structure-based classification and ontology in chemistry. *Journal of Cheminformatics*, **2012**, 4, 8	8.6	31
85	BiNChE: a web tool and library for chemical enrichment analysis based on the ChEBI ontology. *BMC Bioinformatics*, **2015**, 16, 56	3.6	27
84	Synthesis of Carba-Porphyrinoids from Tripyrranes and Unsaturated Dialdehydes. *Synthesis*, **1996**, 1996, 336-340	2.9	27
83	Global open data management in metabolomics. *Current Opinion in Chemical Biology*, **2017**, 36, 58-63	9.7	26
82	Geminal bismethylation prevents polyketide oxidation and dimerization in the benastatin pathway. *Angewandte Chemie - International Edition*, **2007**, 46, 7035-8	16.4	26
81	A database for chemical proteomics: ChEBI. *Methods in Molecular Biology*, **2012**, 803, 273-96	1.4	26
80	Further isoflavonoid metabolites from Millettia griffoniana (Bail). *Phytochemistry*, **2001**, 56, 363-8	4	25
79	Performance validation of neural network based (13)c NMR prediction using a publicly available data source. *Journal of Chemical Information and Modeling*, **2008**, 48, 550-5	6.1	24
78	LUCY: A Program for Structure Elucidation from NMR Correlation Experiments. *Angewandte Chemie International Edition in English*, **1996**, 35, 1984-1986		23
77	The Role of Ionic Backbones in RNA Structure: An Unusually Stable Non-Watson–Crick Duplex of a Nonionic Analog in an Apolar Medium. *Journal of the American Chemical Society*, **1998**, 120, 11576-11580	16.4	22
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, 2015-34	6.1	22

75	Efficient ring perception for the Chemistry Development Kit. *Journal of Cheminformatics*, **2014**, 6, 3	8.6	20
74	New developments on the cheminformatics open workflow environment CDK-Taverna. *Journal of Cheminformatics*, **2011**, 3, 54	8.6	20
73	ChEBI: a chemistry ontology and database. *Journal of Cheminformatics*, **2010**, 2,	8.6	20
72	Identification of Two Chromenes from Calea serrata by Semiautomatic Structure Elucidation. *Journal of Natural Products*, **1997**, 60, 627-628	4.9	19
71	Solution structure of the aminoacyl-capped oligodeoxyribonucleotide duplex (W-TGCGCAC)(2). *Biochemistry*, **1999**, 38, 12597-606	3.2	18
70	The future of metabolomics in ELIXIR. *F1000Research*, **2017**, 6,	3.6	18
69	NaPLeS: a natural products likeness scorer-web application and database. *Journal of Cheminformatics*, **2019**, 11, 55	8.6	17
68	A large-scale protein-function database. *Nature Chemical Biology*, **2010**, 6, 785	11.7	17
67	Metabolomics: The Stethoscope for the Twenty-First Century. *Medical Principles and Practice*, **2021**, 30, 301-310	2.1	17
66	OrChem - An open source chemistry search engine for Oracle(R). *Journal of Cheminformatics*, **2009**, 1, 17	8.6	16
65	Classification and comparison of ligand-binding sites derived from grid-mapped knowledge-based potentials. *Journal of Molecular Graphics and Modelling*, **2006**, 24, 328-40	2.8	16
64	Interoperable and scalable data analysis with microservices: applications in metabolomics. *Bioinformatics*, **2019**, 35, 3752-3760	7.2	15
63	libChEBI: an API for accessing the ChEBI database. *Journal of Cheminformatics*, **2016**, 8, 11	8.6	15
62	Building blocks for automated elucidation of metabolites: natural product-likeness for candidate ranking. *BMC Bioinformatics*, **2014**, 15, 234	3.6	15
61	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	2.3	15
60	The LOTUS Initiative for Open Natural Products Research: Knowledge Management through Wikidata		15
59	So what have data standards ever done for us? The view from metabolomics. *Genome Medicine*, **2010**, 2, 38	14.4	14
58	A lost opportunity for science: journals promote data sharing in metabolomics but do not enforce it. *Metabolomics*, **2018**, 14, 16	4.7	13

57	The Enzyme Portal: a case study in applying user-centred design methods in bioinformatics. *BMC Bioinformatics*, **2013**, 14, 103	3.6	13
56	The EBI enzyme portal. *Nucleic Acids Research*, **2013**, 41, D773-80	20.1	13
55	MASPA Program Predicting Mass Spectra of Combinatorial Libraries. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 449-457		13
54	Self-organizing ontology of biochemically relevant small molecules. *BMC Bioinformatics*, **2012**, 13, 3	3.6	12
53	Evolutionary-algorithm-based strategy for computer-assisted structure elucidation. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 489-98		12
52	DECIMER: towards deep learning for chemical image recognition. *Journal of Cheminformatics*, **2020**, 12, 65	8.6	12
51	In vivo and in vitro identification of Z-BOX C - a new bilirubin oxidation end product. *Organic and Biomolecular Chemistry*, **2018**, 16, 3553-3555	3.9	11
50	MassCascade: Visual Programming for LC-MS Data Processing in Metabolomics. *Molecular Informatics*, **2014**, 33, 307-310	3.8	11
49	Userscripts for the life sciences. *BMC Bioinformatics*, **2007**, 8, 487	3.6	11
48	Too sweet: cheminformatics for deglycosylation in natural products. *Journal of Cheminformatics*, **2020**, 12, 67	8.6	11
47	SpeckTackle: JavaScript charts for spectroscopy. *Journal of Cheminformatics*, **2015**, 7, 17	8.6	10
46	Ten recommendations for software engineering in research. *GigaScience*, **2014**, 3, 31	7.6	10
45	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	3.7	10
44	The future of metabolomics in ELIXIR. *F1000Research*, **2017**, 6, 1649	3.6	10
43	mzML2ISA & nmrML2ISA: generating enriched ISA-Tab metadata files from metabolomics XML data. *Bioinformatics*, **2017**, 33, 2598-2600	7.2	9
42	Metabolic differences in ripening of Solanum lycopersicum 'Ailsa Craig' and three monogenic mutants. *Scientific Data*, **2014**, 1, 140029	8.2	9
41	Alkaloids from Thalictrum przewalskii. *Planta Medica*, **1998**, 64, 165-71	3.1	9
40	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. *Research Ideas and Outcomes*,6,	2.5	9

39	A review of optical chemical structure recognition tools. *Journal of Cheminformatics*, **2020**, 12, 60	8.6	9
38	Automated assembly of species metabolomes through data submission into a public repository. *GigaScience*, **2017**, 6, 1-4	7.6	8
37	A molecular fragment cheminformatics roadmap for mesoscopic simulation. *Journal of Cheminformatics*, **2014**, 6, 45	8.6	8
36	A 4-methyl-7-hydroxyphthalide glycoside and other constituents from Quillaja saponaria molina. *Phytochemistry*, **1995**, 40, 1313-5	4	7
35	Expanding the Rubterolone Family: Intrinsic Reactivity and Directed Diversification of PKS-derived Pyrans. *Chemistry - A European Journal*, **2018**, 24, 11319-11324	4.8	7
34	OntoQuery: easy-to-use web-based OWL querying. *Bioinformatics*, **2013**, 29, 2955-7	7.2	6
33	Metingear: a development environment for annotating genome-scale metabolic models. *Bioinformatics*, **2013**, 29, 2213-5	7.2	6
32	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. *ChemInform*, **2003**, 34, no		6
31	STOUT: SMILES to IUPAC names using neural machine translation. *Journal of Cheminformatics*, **2021** , 13, 34	8.6	6
30	ErtlFunctionalGroupsFinder: automated rule-based functional group detection with the Chemistry Development Kit (CDK). *Journal of Cheminformatics*, **2019**, 11, 37	8.6	5
29	In support of the BMRB. *Nature Structural and Molecular Biology*, **2012**, 19, 854-60	17.6	5
28	Gene Cluster Activation in a Bacterial Symbiont Leads to Halogenated Angucyclic Maduralactomycins and Spirocyclic Actinospirols. *Organic Letters*, **2020**, 22, 2634-2638	6.2	4
27	From Databases to Big Data **2016**, 317-331		4
26	Towards automatic classification within the ChEBI ontology. *Nature Precedings*, **2009**,		4
25	A Catalog of Natural Products Occurring in Watermelon-. *Frontiers in Nutrition*, **2021**, 8, 729822	6.2	3
24	DECIMER 1.0: deep learning for chemical image recognition using transformers. *Journal of Cheminformatics*, **2021**, 13, 61	8.6	3
23	OrChem: an open source chemistry search engine for Oracle. *Journal of Cheminformatics*, **2010**, 2,	8.6	2
22	Progress on an open source computer-assisted structure elucidation suite (SENECA). *Journal of Cheminformatics*, **2010**, 2,	8.6	2

21	Interoperable and scalable data analysis with microservices: Applications in Metabolomics		2
20	Omics Discovery Index - Discovering and Linking Public Omics Datasets		2
19	MAYGEN: an open-source chemical structure generator for constitutional isomers based on the orderly generation principle. *Journal of Cheminformatics*, **2021**, 13, 48	8.6	2
18	ISA API: An open platform for interoperable life science experimental metadata. *GigaScience*, **2021**, 10,	7.6	2
17	Chemical graph generators. *PLoS Computational Biology*, **2021**, 17, e1008504	5	2
16	Computer-Assisted Structure Elucidation1378-1406		2
15	Computational metabolomics a field at the boundaries of cheminformatics and bioinformatics. *Journal of Cheminformatics*, **2011**, 3,	8.6	1
14	Correlations between Chemical Structures and NMR Data **2008**, 1368-1377		1
13	Eine offene NMR-Datenbank. *Nachrichten Aus Der Chemie*, **2005**, 53, 1039-1041	0.1	1
12	PhenoMeNal: Processing and analysis of Metabolomics data in the Cloud		1
11	Accessing and using chemical property databases. *Methods in Molecular Biology*, **2012**, 929, 193-219	1.4	1
10	Description and Analysis of Glycosidic Residues in the Largest Open Natural Products Database. *Biomolecules*, **2021**, 11,	5.9	1
9	DECIMER-Segmentation: Automated extraction of chemical structure depictions from scientific literature. *Journal of Cheminformatics*, **2021**, 13, 20	8.6	1
8	Molecule Set Comparator (MSC): a CDK-based open rich-client tool for molecule set similarity evaluations. *Journal of Cheminformatics*, **2021**, 13, 5	8.6	0
7	Surge: a fast open-source chemical graph generator.. *Journal of Cheminformatics*, **2022**, 14, 24	8.6	0
6	Ontologies in Chemoinformatics **2017**, 2163-2181		
5	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	64.1	
4	Chemical Ontologies for Standardization, Knowledge Discovery, and Data Mining. *Methods and Principles in Medicinal Chemistry*, **2013**, 55-74	0.4	

3 Draft genome assembly and sequencing dataset of the marine diatom cf. RCC75.. *Data in Brief*, **2022**, 41, 107931 1.2

2 Ontologies in Cheminformatics **2016**, 1-19

1 Meet the Editors-in-Chief. *Analytical Science Advances*, **2020**, 1, 4 1.1