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	Performance of chemical structure string representations for chemical image recognition using transformers. , 2022, 1, 84-90.		6
2	Draft genome assembly and sequencing dataset of the marine diatom Skeletonema cf. costatum RCC75. Data in Brief, 2022, 41, 107931.	0.5	1
3	Surge: a fast open-source chemical graph generator. Journal of Cheminformatics, 2022, 14, 24.	2.8	10
4	Notes on the Treatment of Charged Particles for Studying Cyclotide/Membrane Interactions with Dissipative Particle Dynamics. Membranes, 2022, 12, 619.	1.4	0
5	RanDepict: Random chemical structure depiction generator. Journal of Cheminformatics, 2022, 14, .	2.8	3
6	DECIMERâ€”hand-drawn molecule images dataset. Journal of Cheminformatics, 2022, 14, .	2.8	7
7	Metabolomics: The Stethoscope for the Twenty-First Century. Medical Principles and Practice, 2021, 30, 301-310.	1.1	46
8	COCONUT online: Collection of Open Natural Products database. Journal of Cheminformatics, 2021, 13, 2.	2.8	223
9	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
10	Description and Analysis of Glycosidic Residues in the Largest Open Natural Products Database. Biomolecules, 2021, 11, 486.	1.8	4
11	DECIMER-Segmentation: Automated extraction of chemical structure depictions from scientific literature. Journal of Cheminformatics, 2021, 13, 20.	2.8	8
12	STOUT: SMILES to IUPAC names using neural machine translation. Journal of Cheminformatics, 2021, 13, 34.	2.8	25
13	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
14	DECIMER 1.0: deep learning for chemical image recognition using transformers. Journal of Cheminformatics, 2021, 13, 61.	2.8	29
15	ISA API: An open platform for interoperable life science experimental metadata. GigaScience, 2021, 10, .	3.3	19
16	Chemical graph generators. PLoS Computational Biology, 2021, 17, e1008504.	1.5	4
17	A Catalog of Natural Products Occurring in Watermelonâ€”Citrullus lanatus. Frontiers in Nutrition, 2021, 8, 729822.	1.6	4
18	A review of optical chemical structure recognition tools. Journal of Cheminformatics, 2020, 12, 60.	2.8	35

#	Article	IF	Citations
19	Meet the Editors-in-Chief. Analytical Science Advances, 2020, 1, 4.	1.2	0
20	Too sweet: cheminformatics for deglycosylation in natural products. Journal of Cheminformatics, 2020, 12, 67.	2.8	19
21	DECIMER: towards deep learning for chemical image recognition. Journal of Cheminformatics, 2020, 12, 65.	2.8	41
22	Gene Cluster Activation in a Bacterial Symbiont Leads to Halogenated Angucyclic Maduralactomycins and Spirocyclic Actinospirols. Organic Letters, 2020, 22, 2634-2638.	2.4	14
23	Review on natural products databases: where to find data in 2020. Journal of Cheminformatics, 2020, 12, 20.	2.8	243
24	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
25	NFDI4Chem: Shaping a Digital and Cultural Change in Chemistry. Angewandte Chemie - International Edition, 2019, 58, 10766-10768.	7.2	19
26	Automated structure prediction of trans-acyltransferase polyketide synthase products. Nature Chemical Biology, 2019, 15, 813-821.	3.9	94
27	NaPLeS: a natural products likeness scorerâ€"web application and database. Journal of Cheminformatics, 2019, 11, 55.	2.8	28
28	ErtlFunctionalGroupsFinder: automated rule-based functional group detection with the Chemistry Development Kit (CDK). Journal of Cheminformatics, 2019, 11, 37.	2.8	9
29	Interoperable and scalable data analysis with microservices: applications in metabolomics. Bioinformatics, 2019, 35, 3752-3760.	1.8	22
30	NFDI4Chem: Digitalen und kulturellen Wandel in der Chemie gestalten. Angewandte Chemie, 2019, 131, 10880-10882.	1.6	7
31	PhenoMeNal: processing and analysis of metabolomics data in the cloud. GigaScience, 2019, 8, .	3.3	60
32	A lost opportunity for science: journals promote data sharing in metabolomics but do not enforce it. Metabolomics, 2018, 14, 16.	1.4	17
33	In vivoandin vitroidentification ofZ-BOX C â€“ a new bilirubin oxidation end product. Organic and Biomolecular Chemistry, 2018, 16, 3553-3555.	1.5	14
34	NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. Magnetic Resonance in Chemistry, 2018, 56, 703-715.	1.1	61
35	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
36	Expanding the Rubterolone Family: Intrinsic Reactivity and Directed Diversification of PKSâ€derived Pyrans. Chemistry - A European Journal, 2018, 24, 11319-11324.	1.7	15

#	Article	IF	Citations
37	Current Challenges in Plant Eco-Metabolomics. International Journal of Molecular Sciences, 2018, 19, 1385.	1.8	106
38	Frontispiece: Expanding the Rubterolone Family: Intrinsic Reactivity and Directed Diversification of PKS-derived Pyrans. Chemistry - A European Journal, 2018, 24, .	1.7	0
39	Computational tools and workflows in metabolomics: An international survey highlights the opportunity for harmonisation through Galaxy. Metabolomics, 2017, 13, 12.	1.4	69
40	Ontologies in Chemoinformatics. , 2017, , 2163-2181.		0
41	Global open data management in metabolomics. Current Opinion in Chemical Biology, 2017, 36, 58-63.	2.8	39
42	mzML2ISA & nmrML2ISA: generating enriched ISA-Tab metadata files from metabolomics XML data. Bioinformatics, 2017, 33, 2598-2600.	1.8	12
43	Discovering and linking public omics data sets using the Omics Discovery Index. Nature Biotechnology, 2017, 35, 406-409.	9.4	159
44	Automated assembly of species metabolomes through data submission into a public repository. GigaScience, 2017, 6, 1-4.	3.3	9
45	Navigating freely-available software tools for metabolomics analysis. Metabolomics, 2017, 13, 106.	1.4	173
46	Compliance with minimum information guidelines in public metabolomics repositories. Scientific Data, 2017, 4, 170137.	2.4	61
47	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	2.8	275
48	A decade after the metabolomics standards initiative it's time for a revision. Scientific Data, 2017, 4, 170138.	2.4	70
49	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	19
50	The future of metabolomics in ELIXIR. F1000Research, 2017, 6, 1649.	0.8	11
51	The Time Is Right to Focus on Model Organism Metabolomes. Metabolites, 2016, 6, 8.	1.3	63
52	Reaction Decoder Tool (RDT): extracting features from chemical reactions. Bioinformatics, 2016, 32, 2065-2066.	1.8	73
53	ClassyFire: automated chemical classification with a comprehensive, computable taxonomy. Journal of Cheminformatics, 2016, 8, 61.	2.8	779
54	SPLASH, a hashed identifier for mass spectra. Nature Biotechnology, 2016, 34, 1099-1101.	9.4	61

#	Article	IF	Citations
55	libChEBI: an API for accessing the ChEBI database. Journal of Cheminformatics, 2016, 8, 11.	2.8	19
56	MetaboLights: An Openâ€Access Database Repository for Metabolomics Data. Current Protocols in Bioinformatics, 2016, 53, 14.13.1-14.13.18.	25.8	147
57	Data standards can boost metabolomics research, and if there is a will, there is a way. Metabolomics, 2016, 12, 14.	1.4	97
58	From Databases to Big Data. , 2016, , 317-331.		5
59	ChEBI in 2016: Improved services and an expanding collection of metabolites. Nucleic Acids Research, 2016, 44, D1214-D1219.	6.5	752
60	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
61	Ontologies in Cheminformatics. , 2016, , 1-19.		0
62	SpeckTackle: JavaScript charts for spectroscopy. Journal of Cheminformatics, 2015, 7, 17.	2.8	10
63	Updates in Rheaâ€”a manually curated resource of biochemical reactions. Nucleic Acids Research, 2015, 43, D459-D464.	6.5	41
64	COordination of Standards in MetabOlomicS (COSMOS): facilitating integrated metabolomics data access. Metabolomics, 2015, 11, 1587-1597.	1.4	140
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	eNanoMapper: harnessing ontologies to enable data integration for nanomaterial risk assessment. Journal of Biomedical Semantics, 2015, 6, 10.	0.9	63
67	A molecular fragment cheminformatics roadmap for mesoscopic simulation. Journal of Cheminformatics, 2014, 6, 45.	2.8	9
68	Genome-Wide Association Study of Metabolic Traits Reveals Novel Gene-Metabolite-Disease Links. PLoS Genetics, 2014, 10, e1004132.	1.5	86
69	MassCascade: Visual Programming for LCâ€MS Data Processing in Metabolomics. Molecular Informatics, 2014, 33, 307-310.	1.4	12
70	Ten recommendations for software engineering in research. GigaScience, 2014, 3, 31.	3.3	11
71	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
72	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

#	Article	IF	Citations
73	Efficient ring perception for the Chemistry Development Kit. Journal of Cheminformatics, 2014, 6, 3.	2.8	25
74	Building blocks for automated elucidation of metabolites: natural product-likeness for candidate ranking. BMC Bioinformatics, 2014, 15, 234.	1.2	20
75	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
76	Metabolic differences in ripening of Solanum lycopersicum â€˜Ailsa Craigâ€™ and three monogenic mutants. Scientific Data, 2014, 1, 140029.	2.4	12
77	Expanding natural product chemistry resources at the EBI. Journal of Cheminformatics, 2013, 5, .	2.8	0
78	Dissemination of metabolomics results: role of MetaboLights and COSMOS. GigaScience, 2013, 2, 8.	3.3	28
79	The role of reporting standards for metabolite annotation and identification in metabolomic studies. GigaScience, 2013, 2, 13.	3.3	333
80	KNIME-CDK: Workflow-driven cheminformatics. BMC Bioinformatics, 2013, 14, 257.	1.2	119
81	Dovetailing biology and chemistry: integrating the Gene Ontology with the ChEBI chemical ontology. BMC Genomics, 2013, 14, 513.	1.2	45
82	The Enzyme Portal: a case study in applying user-centred design methods in bioinformatics. BMC Bioinformatics, 2013, 14, 103.	1.2	16
83	The EBI enzyme portal. Nucleic Acids Research, 2013, 41, D773-D780.	6.5	19
84	MetaboLightsâ€”an open-access general-purpose repository for metabolomics studies and associated meta-data. Nucleic Acids Research, 2013, 41, D781-D786.	6.5	578
85	The MetaboLights repository: curation challenges in metabolomics. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat029.	1.4	46
86	OntoQuery: easy-to-use web-based OWL querying. Bioinformatics, 2013, 29, 2955-2957.	1.8	7
87	Metingear: a development environment for annotating genome-scale metabolic models. Bioinformatics, 2013, 29, 2213-2215.	1.8	7
88	LipidHome: A Database of Theoretical Lipids Optimized for High Throughput Mass Spectrometry Lipidomics. PLoS ONE, 2013, 8, e61951.	1.1	69
89	Bioinformatics Meets User-Centred Design: A Perspective. PLoS Computational Biology, 2012, 8, e1002554.	1.5	50
90	The ChEBI reference database and ontology for biologically relevant chemistry: enhancements for 2013. Nucleic Acids Research, 2012, 41, D456-D463.	6.5	508

#	Article	IF	Citations
91	Rheaâ€"a manually curated resource of biochemical reactions. Nucleic Acids Research, 2012, 40, D754-D760.	6.5	84
92	Toward interoperable bioscience data. Nature Genetics, 2012, 44, 121-126.	9.4	362
93	MetaboLights: towards a new COSMOS of metabolomics data management. Metabolomics, 2012, 8, 757-760.	1.4	79
94	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
95	Natural product-likeness score revisited: an open-source, open-data implementation. BMC Bioinformatics, 2012, 13, 106.	1.2	63
96	Self-organizing ontology of biochemically relevant small molecules. BMC Bioinformatics, 2012, 13, 3.	1.2	20
97	Structure-based classification and ontology in chemistry. Journal of Cheminformatics, 2012, 4, 8.	2.8	40
98	In support of the BMRB. Nature Structural and Molecular Biology, 2012, 19, 854-860.	3.6	6
99	Structured chemical class definitions and automated matching for chemical ontology evolution. Journal of Cheminformatics, 2012, 4, .	2.8	0
100	A Database for Chemical Proteomics: ChEBI. Methods in Molecular Biology, 2012, 803, 273-296.	0.4	26
101	Accessing and Using Chemical Property Databases. Methods in Molecular Biology, 2012, 929, 193-219.	0.4	1
102	Minimum information about a bioactive entity (MIABE). Nature Reviews Drug Discovery, 2011, 10, 661-669.	21.5	80
103	New developments on the cheminformatics open workflow environment CDK-Taverna. Journal of Cheminformatics, 2011, 3, 54.	2.8	23
104	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
105	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	2.8	63
106	Computational metabolomics â€" a field at the boundaries of cheminformatics and bioinformatics. Journal of Cheminformatics, 2011, 3, .	2.8	1
107	The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web. PLoS ONE, 2011, 6, e25513.	1.1	86
108	CDK-Taverna: an open workflow environment for cheminformatics. BMC Bioinformatics, 2010, 11, 159.	1.2	54

#	Article	IF	Citations
109	OrChem: an open source chemistry search engine for Oracle. Journal of Cheminformatics, 2010, 2, .	2.8	2
110	Progress on an open source computer-assisted structure elucidation suite (SENECA). Journal of Cheminformatics, 2010, 2, .	2.8	2
111	ChEBI: a chemistry ontology and database. Journal of Cheminformatics, 2010, 2, .	2.8	22
112	A large-scale protein-function database. Nature Chemical Biology, 2010, 6, 785-785.	3.9	22
113	ChEBI â€“ an Open-access Chemistry Resource for the Life Sciences:*Facilities for On-line Submission and Curation. Nature Precedings, 2010, , .	0.1	0
114	Chemical Entities of Biological Interest: an update. Nucleic Acids Research, 2010, 38, D249-D254.	6.5	248
115	So what have data standards ever done for us? The view from metabolomics. Genome Medicine, 2010, 2, 38.	3.6	19
116	Towards automatic classification within the ChEBI ontology. Nature Precedings, 2009, , .	0.1	4
117	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	1.2	52
118	OrChem - An open source chemistry search engine for OracleÂ®. Journal of Cheminformatics, 2009, 1, 17.	2.8	18
119	Creating chemo- & bioinformatics workflows, further developments within the CDK-Taverna Project. Chemistry Central Journal, 2008, 2, .	2.6	0
120	Building blocks for automated elucidation of metabolites: Machine learning methods for NMR prediction. BMC Bioinformatics, 2008, 9, 400.	1.2	97
121	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
122	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
123	Geminal Bismethylation Prevents Polyketide Oxidation and Dimerization in the Benastatin Pathway. Angewandte Chemie - International Edition, 2007, 46, 7035-7038.	7.2	28
124	Userscripts for the Life Sciences. BMC Bioinformatics, 2007, 8, 487.	1.2	14
125	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	1.2	111
126	The Blue Obeliskâ€”Interoperability in Chemical Informatics. Journal of Chemical Information and Modeling, 2006, 46, 991-998.	2.5	366

#	Article	IF	Citations
127	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
128	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
129	Eine offene NMRâ€Datenbank. Nachrichten Aus Der Chemie, 2005, 53, 1039-1041.	0.0	1
130	Evolutionary-Algorithm-Based Strategy for Computer-Assisted Structure Elucidation.. ChemInform, 2004, 35, no.	0.1	0
131	Recent Developments in Automated Structure Elucidation of Natural Products. ChemInform, 2004, 35, no.	0.1	0
132	NMRShiftDB â€“ compound identification and structure elucidation support through a free community-built web database. Phytochemistry, 2004, 65, 2711-2717.	1.4	113
133	Recent developments in automated structure elucidation of natural products. Natural Product Reports, 2004, 21, 512.	5.2	86
134	Evolutionary-Algorithm-Based Strategy for Computer-Assisted Structure Elucidation. Journal of Chemical Information and Computer Sciences, 2004, 44, 489-498.	2.8	20
135	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
136	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. ChemInform, 2003, 34, no.	0.1	9
137	NMRShiftDBConstructing a Free Chemical Information System with Open-Source Components. Journal of Chemical Information and Computer Sciences, 2003, 43, 1733-1739.	2.8	127
138	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
139	Further isoflavonoid metabolites from Millettia griffoniana (Bail). Phytochemistry, 2001, 56, 363-368.	1.4	31
140	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
141	Solution Structure of the Aminoacyl-Capped Oligodeoxyribonucleotide Duplex (W-TGCGCAC)2â€. Biochemistry, 1999, 38, 12597-12606.	1.2	19
142	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
143	Alkaloids fromThalictrum przewalskii. Planta Medica, 1998, 64, 165-171.	0.7	11
144	MASPA Program Predicting Mass Spectra of Combinatorial Libraries. Journal of Chemical Information and Computer Sciences, 1997, 37, 449-457.	2.8	15

#	Article	IF	Citations
145	Identification of Two Chromenes fromCalea serrataby Semiautomatic Structure Elucidation. Journal of Natural Products, 1997, 60, 627-628.	1.5	21
146	Spectrometrically monitored selection experiments: quantitative laser desorption mass spectrometry of small chemical libraries. Chemistry and Biology, 1997, 4, 63-77.	6.2	39
147	LUCYâ€"A Program for Structure Elucidation from NMR Correlation Experiments. Angewandte Chemie International Edition in English, 1996, 35, 1984-1986.	4.4	26
148	Synthesis of Carba-Porphyrinoids from Tripyrranes and Unsaturated Dialdehydes. Synthesis, 1996, 1996, 336-340.	1.2	35
149	Alkaloids from Dactylicapnos torulosa. Phytochemistry, 1995, 40, 299-305.	1.4	44
150	A 4-methyl-7-hydroxyphthalide glycoside and other constituents from Quillaja saponaria molina. Phytochemistry, 1995, 40, 1313-1315.	1.4	11
151	NFDI4Chem - Towards a National Research Data Infrastructure for Chemistry in Germany. Research Ideas and Outcomes, 0, 6, .	1.0	25
152	The LOTUS initiative for open knowledge management in natural products research. ELife, 0, 11, .	2.8	90