Stefan Kuhn

List of Publications by Year
in descending order

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44 papers	2,666 citations	535685 17 h-index	263392 45 g-index
50 all docs	50 docs citations	50 times ranked	3730 citing authors

#	Article	IF	Citations
1	A dataâ€oriented approach to making new molecules as a student experiment: artificial intelligenceâ€enabling FAIR publication of NMR data for organic esters. Magnetic Resonance in Chemistry, 2022, 60, 93-103.	1.1	9
2	A pilot study for fragment identification using 2D NMR and deep learning. Magnetic Resonance in Chemistry, 2022, 60, 1052-1060.	1.1	9
3	Computational simulation of ¹H NMR profiles of complex biofluid analyte mixtures at differential operating frequencies: Applications to lowâ€field benchtop spectra. Magnetic Resonance in Chemistry, 2022, 60, 1097-1112.	1.1	6
4	Prediction of chemical shift in NMR: A review. Magnetic Resonance in Chemistry, 2022, 60, 1021-1031.	1.1	38
5	A Proposed VR Platform for Supporting Blended Learning Post COVID-19. Education Sciences, 2022, 12, 435.	1.4	7
6	Combining high-speed countercurrent chromatography three-phase solvent system with electrospray ionization-mass spectrometry and nuclear magnetic resonance to profile the unconventional food plant Syzygium malaccense. Journal of Chromatography A, 2022, 1677, 463211.	1.8	5
7	Modelling of DNA mismatch repair with a reversible process calculus. Theoretical Computer Science, 2022, 925, 68-86.	0.5	1
8	Data format standards in analytical chemistry. Pure and Applied Chemistry, 2022, 94, 725-736.	0.9	4
9	Reversibility of Executable Interval Temporal Logic Specifications. Lecture Notes in Computer Science, 2021, , 214-223.	1.0	1
10	The Three Pillars of Natural Product Dereplication. Alkaloids from the Bulbs of Urceolina peruviana (C. Presl) J.F. Macbr. as a Preliminary Test Case. Molecules, 2021, 26, 637.	1.7	16
11	NMReDATA: Tools and applications. Magnetic Resonance in Chemistry, 2021, 59, 792-803.	1.1	12
12	Evolving Deep Learning Convolutional Neural Networks for Early COVID-19 Detection in Chest X-ray Images. Mathematics, 2021, 9, 1002.	1.1	37
13	SCIPS: A serious game using a guidance mechanic to scaffold effective training for cyber security. Information Sciences, 2021, 580, 524-540.	4.0	7
14	Shallow buried improvised explosive device detection via convolutional neural networks. Integrated Computer-Aided Engineering, 2020, 27, 403-416.	2.5	11
15	Applying NMR compound identification using NMRfilter to match predicted to experimental data. Metabolomics, 2020, 16, 123.	1.4	15
16	Identifying Parkinsonâ€™s Disease Through the Classification of Audio Recording Data. , 2020, , .		5
17	A Neural Network for Interpolating Light-Sources. , 2020, , .		0
18	Reversibility in Chemical Reactions. Lecture Notes in Computer Science, 2020, , 151-176.	1.0	8

#	Article	IF	Citations
19	Data mining and visualisation: general discussion. Faraday Discussions, 2019, 218, 354-371.	1.6	2
20	Future challenges and new approaches: general discussion. Faraday Discussions, 2019, 218, 505-523.	1.6	1
21	Rapid prediction of NMR spectral properties with quantified uncertainty. Journal of Cheminformatics, 2019, 11, 50.	2.8	57
22	Stereo-Aware Extension of HOSE Codes. ACS Omega, 2019, 4, 7323-7329.	1.6	22
23	An integrated approach for mixture analysis using MS and NMR techniques. Faraday Discussions, 2019, 218, 339-353.	1.6	22
24	Puffle-Pod Marine Evacuation System (POMES). , 2019, , .		0
25	NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. Magnetic Resonance in Chemistry, 2018, 56, 703-715.	1.1	61
26	Local reversibility in a Calculus of Covalent Bonding. Science of Computer Programming, 2018, 151, 18-47.	1.5	14
27	The C6H6 NMR repository: An integral solution to control the flow of your data from the magnet to the public. Magnetic Resonance in Chemistry, 2018, 56, 520-528.	1.1	19
28	Simulation of Base Excision Repair in the Calculus of Covalent Bonding. Lecture Notes in Computer Science, 2018, , 123-129.	1.0	2
29	The Chemistry Development Kit (CDK) v2.0: atom typing, depiction, molecular formulas, and substructure searching. Journal of Cheminformatics, 2017, 9, 33.	2.8	275
30	A Calculus for Local Reversibility. Lecture Notes in Computer Science, 2016, , 20-35.	1.0	11
31	Facilitating quality control for spectra assignments of small organic molecules: nmrshiftdb2 â€“ a free inâ€house NMR database with integrated LIMS for academic service laboratories. Magnetic Resonance in Chemistry, 2015, 53, 582-589.	1.1	83
32	From chemical shift data through prediction to assignment and NMR LIMS - multiple functionalities of nmrshiftdb2. Journal of Cheminformatics, 2012, 4, .	2.8	12
33	Computational metabolomics â€“ a field at the boundaries of cheminformatics and bioinformatics. Journal of Cheminformatics, 2011, 3, .	2.8	1
34	Progress on an open source computer-assisted structure elucidation suite (SENECA). Journal of Cheminformatics, 2010, 2, .	2.8	2
35	Bioclipse 2: A scriptable integration platform for the life sciences. BMC Bioinformatics, 2009, 10, 397.	1.2	52
36	Building blocks for automated elucidation of metabolites: Machine learning methods for NMR prediction. BMC Bioinformatics, 2008, 9, 400.	1.2	97

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37	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
38	Bioclipse: an open source workbench for chemo- and bioinformatics. BMC Bioinformatics, 2007, 8, 59.	1.2	111
39	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
40	Eine offene NMRâ€Datenbank. Nachrichten Aus Der Chemie, 2005, 53, 1039-1041.	0.0	1
41	NMRShiftDB â€“ compound identification and structure elucidation support through a free community-built web database. Phytochemistry, 2004, 65, 2711-2717.	1.4	113
42	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
43	The Chemistry Development Kit (CDK): An Open-Source Java Library for Chemo- and Bioinformatics.. ChemInform, 2003, 34, no.	0.1	9
44	NMRShiftDBConstructing a Free Chemical Information System with Open-Source Components. Journal of Chemical Information and Computer Sciences, 2003, 43, 1733-1739.	2.8	127