Antony John Williams

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/3673325/publications.pdf

Version: 2024-02-01

262 papers	12,714 citations	28190 55 h-index	31759 101 g-index
284 all docs	284 docs citations	284 times ranked	11409 citing authors

#	Article	IF	Citations
1	ChemSpider: An Online Chemical Information Resource. Journal of Chemical Education, 2010, 87, 1123-1124.	1.1	848
2	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Journal of Cheminformatics, 2017, 9, 61.	2.8	674
3	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. Chemical Research in Toxicology, 2016, 29, 1225-1251.	1.7	456
4	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	1.3	453
5	Comparison of Different Approaches to Define the Applicability Domain of QSAR Models. Molecules, 2012, 17, 4791-4810.	1.7	370
6	OPERA models for predicting physicochemical properties and environmental fate endpoints. Journal of Cheminformatics, 2018, 10, 10.	2.8	326
7	Open PHACTS: semantic interoperability for drug discovery. Drug Discovery Today, 2012, 17, 1188-1198.	3.2	274
8	In silico repositioning of approved drugs for rare and neglected diseases. Drug Discovery Today, 2011, 16, 298-310.	3.2	269
9	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. Environmental Health Perspectives, 2016, 124, 1023-1033.	2.8	264
10	Integrated Model of Chemical Perturbations of a Biological Pathway Using 18In VitroHigh-Throughput Screening Assays for the Estrogen Receptor. Toxicological Sciences, 2015, 148, 137-154.	1.4	251
11	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. Toxicological Sciences, 2019, 169, 317-332.	1.4	225
12	Major Structural Components in Freshwater Dissolved Organic Matter. Environmental Science & Technology, 2007, 41, 8240-8247.	4.6	223
13	A bibliometric review of drug repurposing. Drug Discovery Today, 2018, 23, 661-672.	3.2	163
14	Quantitative Structureâ€“Activity Relationship Models for Ready Biodegradability of Chemicals. Journal of Chemical Information and Modeling, 2013, 53, 867-878.	2.5	160
15	Integrating tools for non-targeted analysis research and chemical safety evaluations at the US EPA. Journal of Exposure Science and Environmental Epidemiology, 2018, 28, 411-426.	1.8	148
16	Identification of â€œKnown Unknownsâ€•Utilizing Accurate Mass Data and ChemSpider. Journal of the American Society for Mass Spectrometry, 2012, 23, 179-185.	1.2	145
17	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. Chemical Research in Toxicology, 2021, 34, 189-216.	1.7	145
18	Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring. Environment International, 2016, 88, 269-280.	4.8	143

#	Article	IF	Citations
19	Computer-assisted structure verification and elucidation tools in NMR-based structure elucidation. Progress in Nuclear Magnetic Resonance Spectroscopy, 2008, 53, 1-104.	3.9	135
20	The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products. Scientific Data, 2018, 5, 180125.	2.4	132
21	EPAâ€™s DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. Computational Toxicology, 2019, 12, 100096.	1.8	127
22	Predicting Hepatotoxicity Using ToxCast in Vitro Bioactivity and Chemical Structure. Chemical Research in Toxicology, 2015, 28, 738-751.	1.7	124
23	Smart Phones, a Powerful Tool in the Chemistry Classroom. Journal of Chemical Education, 2011, 88, 683-686.	1.1	120
24	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
25	EPAâ€™s non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings. Analytical and Bioanalytical Chemistry, 2019, 411, 853-866.	1.9	116
26	A Predictive Ligand-Based Bayesian Model for Human Drug-Induced Liver Injury. Drug Metabolism and Disposition, 2010, 38, 2302-2308.	1.7	106
27	In Silico Prediction of Physicochemical Properties of Environmental Chemicals Using Molecular Fingerprints and Machine Learning. Journal of Chemical Information and Modeling, 2017, 57, 36-49.	2.5	106
28	Exposome-Scale Investigations Guided by Global Metabolomics, Pathway Analysis, and Cognitive Computing. Analytical Chemistry, 2017, 89, 11505-11513.	3.2	106
29	Towards a gold standard: regarding quality in public domain chemistry databases and approaches to improving the situation. Drug Discovery Today, 2012, 17, 685-701.	3.2	102
30	The ChEMBL database as linked open data. Journal of Cheminformatics, 2013, 5, 23.	2.8	96
31	Structural revisions of natural products by Computer-Assisted Structure Elucidation (CASE) systems. Natural Product Reports, 2010, 27, 1296.	5.2	95
32	A Combined Atomic Force Microscopy and Computational Approach for the Structural Elucidation of Breitfussin A and B: Highly Modified Halogenated Dipeptides from Thuiaria breitfussi. Angewandte Chemie - International Edition, 2012, 51, 12238-12241.	7.2	92
33	Suspect screening and non-targeted analysis of drinking water using point-of-use filters. Environmental Pollution, 2018, 234, 297-306.	3.7	90
34	Open-source QSAR models for pKa prediction using multiple machine learning approaches. Journal of Cheminformatics, 2019, 11, 60.	2.8	90
35	An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling. SAR and QSAR in Environmental Research, 2016, 27, 911-937.	1.0	89
36	Identifying known unknowns using the US EPAâ€™s CompTox Chemistry Dashboard. Analytical and Bioanalytical Chemistry, 2017, 409, 1729-1735.	1.9	89

#	Article	IF	Citations
37	A quality alert and call for improved curation of public chemistry databases. Drug Discovery Today, 2011, 16, 747-750.	3.2	88
38	Suspect Screening Analysis of Chemicals in Consumer Products. Environmental Science & Technology, 2018, 52, 3125-3135.	4.6	88
39	Carbon-carbon double-bond formation in the intermolecular acetonitrile reductive coupling promoted by a mononuclear titanium(II) compound. Preparation and characterization of two titanium(IV) imido derivatives. Inorganic Chemistry, 1991, 30, 4863-4866.	1.9	81
40	Improved Baseline Recognition and Modeling of FT NMR Spectra. Journal of Magnetic Resonance, 2000, 146, 122-125.	1.2	79
41	Development and Application of Liquid Chromatographic Retention Time Indices in HRMS-Based Suspect and Nontarget Screening. Analytical Chemistry, 2021, 93, 11601-11611.	3.2	79
42	Structure Elucidator:â€‰A Versatile Expert System for Molecular Structure Elucidation from 1D and 2D NMR Data and Molecular Fragments. Journal of Chemical Information and Computer Sciences, 2004, 44, 771-792.	2.8	78
43	A Chemical Category-Based Prioritization Approach for Selecting 75 Per- and Polyfluoroalkyl Substances (PFAS) for Tiered Toxicity and Toxicokinetic Testing. Environmental Health Perspectives, 2019, 127, 14501.	2.8	75
44	Internet-based tools for communication and collaboration in chemistry. Drug Discovery Today, 2008, 13, 502-506.	3.2	71
45	Assessing the organic composition of urban surface films using nuclear magnetic resonance spectroscopy. Chemosphere, 2006, 63, 142-152.	4.2	65
46	The Application of1H High-Resolution Magic-Angle Spinning NMR for the Study of Clayâ^'Organic Associations in Natural and Synthetic Complexes. Langmuir, 2006, 22, 4498-4503.	1.6	64
47	The use of NMR to study sodium dodecyl sulfate-gelatin interactions. Langmuir, 1994, 10, 68-71.	1.6	63
48	Application of a New Expert System for the Structure Elucidation of Natural Products from Their 1D and 2D NMR Data. Journal of Natural Products, 2002, 65, 693-703.	1.5	63
49	A perspective of publicly accessible/open-access chemistry databases. Drug Discovery Today, 2008, 13, 495-501.	3.2	63
50	Precompetitive preclinical ADME/Tox data: set it free on the web to facilitate computational model building and assist drug development. Lab on A Chip, 2010, 10, 13-22.	3.1	63
51	Computer-assisted structure elucidation of natural products with limited 2D NMR data: application of the StrucEluc system. Magnetic Resonance in Chemistry, 2003, 41, 359-372.	1.1	61
52	Toward More Reliable ¹³C and ¹H Chemical Shift Prediction:â€‰ A Systematic Comparison of Neural-Network and Least-Squares Regression Based Approaches. Journal of Chemical Information and Modeling, 2008, 48, 128-134.	2.5	61
53	NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. Magnetic Resonance in Chemistry, 2018, 56, 703-715.	1.1	61
54	The development of models to predict melting and pyrolysis point data associated with several hundred thousand compounds mined from PATENTS. Journal of Cheminformatics, 2016, 8, 2.	2.8	60

#	Article	IF	Citations
55	â€œMS-Readyâ€•structures for non-targeted high-resolution mass spectrometry screening studies. Journal of Cheminformatics, 2018, 10, 45.	2.8	59
56	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. Toxicology, 2021, 457, 152789.	2.0	57
57	Combined x-ray crystallographic, single-crystal EPR, and theoretical study of metal-centered radicals of the type [.eta.5C5R5Cr(CO)2L] (R = H, Me; L = CO, tertiary phosphine). Journal of the American Chemical Society, 1991, 113, 542-551.	6.6	55
58	Facile Rearrangements of Alkynylamino Heterocycles with Noble Metal Cations. Journal of Organic Chemistry, 1996, 61, 3289-3297.	1.7	54
59	Identification of degradants of a complex alkaloid using NMR cryoprobe technology and ACD/structure elucidator. Journal of Heterocyclic Chemistry, 2002, 39, 1241-1250.	1.4	54
60	Computer-assisted methods for molecular structure elucidation: realizing a spectroscopist's dream. Journal of Cheminformatics, 2009, 1, 3.	2.8	54
61	Using prepared mixtures of ToxCast chemicals to evaluate non-targeted analysis (NTA) method performance. Analytical and Bioanalytical Chemistry, 2019, 411, 835-851.	1.9	54
62	Open Science for Identifying â€œKnown Unknownâ€•Chemicals. Environmental Science & Technology, 2017, 51, 5357-5359.	4.6	53
63	Reaching Out to Collaborators: Crowdsourcing for Pharmaceutical Research. Pharmaceutical Research, 2010, 27, 393-395.	1.7	52
64	Long-range carbon-carbon connectivity via unsymmetrical indirect covariance processing of HSQC and HMBC NMR data. Magnetic Resonance in Chemistry, 2006, 44, 107-109.	1.1	51
65	Identifying residues in natural organic matter through spectral prediction and pattern matching of 2D NMR datasets. Magnetic Resonance in Chemistry, 2004, 42, 14-22.	1.1	50
66	Open drug discovery for the Zika virus. F1000Research, 2016, 5, 150.	0.8	50
67	Predicting Organ Toxicity Using in Vitro Bioactivity Data and Chemical Structure. Chemical Research in Toxicology, 2017, 30, 2046-2059.	1.7	49
68	A comparison of three liquid chromatography (LC) retention time prediction models. Talanta, 2018, 182, 371-379.	2.9	49
69	Finding Promiscuous Old Drugs for New Uses. Pharmaceutical Research, 2011, 28, 1785-1791.	1.7	48
70	FluoroMatch 2.0â€”making automated and comprehensive non-targeted PFAS annotation a reality. Analytical and Bioanalytical Chemistry, 2022, 414, 1201-1215.	1.9	48
71	Programmatic conversion of crystal structures into 3D printable files using Jmol. Journal of Cheminformatics, 2016, 8, 66.	2.8	46
72	Progress towards an OECD reporting framework for transcriptomics and metabolomics in regulatory toxicology. Regulatory Toxicology and Pharmacology, 2021, 125, 105020.	1.3	46

#	Article	IF	Citations
73	The Royal Society of Chemistry and the delivery of chemistry data repositories for the community. Journal of Computer-Aided Molecular Design, 2014, 28, 1023-1030.	1.3	45
74	Abstract Sifter: a comprehensive front-end system to PubMed. F1000Research, 2017, 6, 2164.	0.8	45
75	Unsymmetrical covariance processing of COSY or TOCSY and HSQC NMR data to obtain the equivalent of HSQCâ€COSY or HSQCâ€TOCSY spectra. Journal of Heterocyclic Chemistry, 2006, 43, 163-166.	1.4	44
76	The Spectral Game: leveraging Open Data and crowdsourcing for education. Journal of Cheminformatics, 2009, 1, 9.	2.8	44
77	Mobile apps for chemistry in the world of drug discovery. Drug Discovery Today, 2011, 16, 928-939.	3.2	44
78	Scientific competency questions as the basis for semantically enriched open pharmacological space development. Drug Discovery Today, 2013, 18, 843-852.	3.2	44
79	An expert system for automated structure elucidation utilizing 1 H- 1 H, 13 C- 1 H and 15 N- 1 H 2D NMR correlations. Fresenius' Journal of Analytical Chemistry, 2001, 369, 709-714.	1.5	41
80	Structure Elucidation from 2D NMR Spectra Using theStrucElucExpert System:â€‰ Detection and Removal of Contradictions in the Data. Journal of Chemical Information and Computer Sciences, 2004, 44, 1737-1751.	2.8	41
81	Looking Back to the Future: Predicting in Vivo Efficacy of Small Molecules versus Mycobacterium tuberculosis. Journal of Chemical Information and Modeling, 2014, 54, 1070-1082.	2.5	41
82	Applying linked data approaches to pharmacology: Architectural decisions and implementation. Semantic Web, 2014, 5, 101-113.	1.1	41
83	Lowâ€Energy, Largeâ€Angle Electronâ€Impact Spectra: Helium, Nitrogen, Ethylene, and Benzene. Journal of Chemical Physics, 1967, 47, 4180-4185.	1.2	40
84	Development of a fast and accurate method of 13C NMR chemical shift prediction. Chemometrics and Intelligent Laboratory Systems, 2009, 97, 91-97.	1.8	40
85	Quindolinocryptotackieine: the elucidation of a novel indoloquinoline alkaloid structure through the use of computer-assisted structure elucidation and 2D NMR. Magnetic Resonance in Chemistry, 2003, 41, 577-584.	1.1	39
86	Are Deterministic Expert Systems for Computer-Assisted Structure Elucidation Obsolete?. Journal of Chemical Information and Modeling, 2006, 46, 1643-1656.	2.5	39
87	Incorporating Green Chemistry Concepts into Mobile Chemistry Applications and Their Potential Uses. ACS Sustainable Chemistry and Engineering, 2013, 1, 8-13.	3.2	39
88	The Synthesis and STM/AFM Imaging of â€˜Olympiceneâ€™ Benzo[cd]pyrenes. Chemistry - A European Journal, 2015, 21, 2011-2018.	1.7	39
89	Dispensing Processes Impact Apparent Biological Activity as Determined by Computational and Statistical Analyses. PLoS ONE, 2013, 8, e62325.	1.1	39
90	Empirical and DFT GIAO quantumâ€mechanical methods of ¹³C chemical shifts prediction: competitors or collaborators?. Magnetic Resonance in Chemistry, 2010, 48, 219-229.	1.1	37

#	Article	IF	Citations
91	Microstructure analysis at the percolation threshold in reverse microemulsions. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 1997, 128, 1-11.	2.3	36
92	When pharmaceutical companies publish large datasets: an abundance of riches or fool's gold?. Drug Discovery Today, 2010, 15, 812-815.	3.2	36
93	Enabling High-Throughput Searches for Multiple Chemical Data Using the U.S.-EPA CompTox Chemicals Dashboard. Journal of Chemical Information and Modeling, 2021, 61, 565-570.	2.5	36
94	Systematic Evidence Map for Over One Hundred and Fifty Per- and Polyfluoroalkyl Substances (PFAS). Environmental Health Perspectives, 2022, 130, 56001.	2.8	36
95	Fuzzy Structure Generation:â€‰ A New Efficient Tool for Computer-Aided Structure Elucidation (CASE). Journal of Chemical Information and Modeling, 2007, 47, 1053-1066.	2.5	35
96	Computer-aided determination of relative stereochemistry and 3D models of complex organic molecules from 2D NMR spectra. Tetrahedron, 2005, 61, 9980-9989.	1.0	34
97	Analysis and elimination of artifacts in indirect covariance NMR spectra via unsymmetrical processing. Magnetic Resonance in Chemistry, 2005, 43, 999-1007.	1.1	34
98	NMR relaxation studies of internal motions: a comparison between micelles and related systems. The Journal of Physical Chemistry, 1990, 94, 2727-2729.	2.9	33
99	The use of unsymmetrical indirect covariance NMR methods to obtain the equivalent of HSQC-NOESY data. Magnetic Resonance in Chemistry, 2007, 45, 544-546.	1.1	33
100	Automatic vs. manual curation of a multi-source chemical dictionary: the impact on text mining. Journal of Cheminformatics, 2010, 2, 3.	2.8	33
101	Sourcing data on chemical properties and hazard data from the US-EPA CompTox Chemicals Dashboard: A practical guide for human risk assessment. Environment International, 2021, 154, 106566.	4.8	33
102	Long-Range 1Hâ€“15N Heteronuclear Shift Correlation. Annual Reports on NMR Spectroscopy, 2005, 55, 1-119.	0.7	32
103	Utilizing unsymmetrical indirect covariance processing to define15Nï£¿13C connectivity networks. Magnetic Resonance in Chemistry, 2007, 45, 624-627.	1.1	32
104	Open Drug Discovery Teams: A Chemistry Mobile App for Collaboration. Molecular Informatics, 2012, 31, 585-597.	1.4	32
105	Four disruptive strategies for removing drug discovery bottlenecks. Drug Discovery Today, 2013, 18, 265-271.	3.2	32
106	Weaver's historic accessible collection of synthetic dyes: a cheminformatics analysis. Chemical Science, 2017, 8, 4334-4339.	3.7	32
107	An x-ray crystallographic and single-crystal EPR investigation of the cationic, iron-centered radical tricarbonylbis(triphenylphosphine)iron(I), {Fe(CO)3(PPh3)2+}. A theoretical examination of the structural preferences of five-coordinated seventeen-electron complexes. Journal of the American Chemical Society, 1991, 113, 9834-9842.	6.6	31
108	In silico MS/MS spectra for identifying unknowns: a critical examination using CFM-ID algorithms and ENTACT mixture samples. Analytical and Bioanalytical Chemistry, 2020, 412, 1303-1315.	1.9	31

#	Article	IF	Citations
109	Automated structure verification based on a combination of 1D ¹H NMR and 2D ¹Hï£¿¹³C HSQC spectra. Magnetic Resonance in Chemistry, 2007, 45, 803-813.	1.1	30
110	Annotating Human Pâ€Glycoprotein Bioassay Data. Molecular Informatics, 2012, 31, 599-609.	1.4	30
111	Structure Revision of Asperjinone Using Computer-Assisted Structure Elucidation Methods. Journal of Natural Products, 2013, 76, 113-116.	1.5	30
112	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. Future Medicinal Chemistry, 2015, 7, 1921-1936.	1.1	30
113	Chemical Characterization of Recycled Consumer Products Using Suspect Screening Analysis. Environmental Science & Technology, 2021, 55, 11375-11387.	4.6	30
114	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
115	Assessing bioaccumulation of polybrominated diphenyl ethers for aquatic species by QSAR modeling. Chemosphere, 2012, 89, 433-444.	4.2	28
116	Parallel Worlds of Public and Commercial Bioactive Chemistry Data. Journal of Medicinal Chemistry, 2015, 58, 2068-2076.	2.9	28
117	Big Data and Chemical Education. Journal of Chemical Education, 2016, 93, 504-508.	1.1	28
118	Linking in silico MS/MS spectra with chemistry data to improve identification of unknowns. Scientific Data, 2019, 6, 141.	2.4	28
119	Automated structure verification based on1H NMR prediction. Magnetic Resonance in Chemistry, 2006, 44, 524-538.	1.1	27
120	A systematic approach for the generation and verification of structural hypotheses. Magnetic Resonance in Chemistry, 2009, 47, 371-389.	1.1	27
121	Computerâ€“Based Structure Elucidation from Spectral Data. Lecture Notes in Quantum Chemistry II, 2015, , .	0.3	27
122	Lowâ€Energy Electronâ€Impact Study of the 12â€“14â€eV Transitions in Nitrogen. Journal of Chemical Physics, 1969, 51, 2859-2865.	1.2	26
123	Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data. Journal of Cheminformatics, 2015, 7, 9.	2.8	26
124	Prediction of Estrogenic Bioactivity of Environmental Chemical Metabolites. Chemical Research in Toxicology, 2016, 29, 1410-1427.	1.7	26
125	Isolated free-radical pairs in Rb+ 18-crown-6 TCNQ? single crystals (TCNQ =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 102 Td (te	2.0	25
126	Applying Computer-Assisted Structure Elucidation Algorithms for the Purpose of Structure Validation: Revisiting the NMR Assignments of Hexacyclinol. Journal of Natural Products, 2008, 71, 581-588.	1.5	25

#	Article	IF	Citations
127	Redefining Cheminformatics with Intuitive Collaborative Mobile Apps. Molecular Informatics, 2012, 31, 569-584.	1.4	25
128	Evaluating opportunities for advancing the use of alternative methods in risk assessment through the development of fit-for-purpose in vitro assays. Toxicology in Vitro, 2018, 48, 310-317.	1.1	25
129	Challenges and recommendations for obtaining chemical structures of industry-provided repurposing candidates. Drug Discovery Today, 2013, 18, 58-70.	3.2	24
130	Predictive Structure-Based Toxicology Approaches To Assess the Androgenic Potential of Chemicals. Journal of Chemical Information and Modeling, 2017, 57, 2874-2884.	2.5	24
131	Exchange processes in diselenium and selenium-sulfur dihalides, Se2X2 and SeSX2 (X = Br, Cl). A selenium-77 2D-EXSY study. Inorganic Chemistry, 1992, 31, 4534-4538.	1.9	23
132	Using Unsymmetrical Indirect Covariance Processing to Calculate GHSQC-COSY Spectra. Journal of Natural Products, 2007, 70, 1393-1396.	1.5	23
133	Meta-analysis of molecular property patterns and filtering of public datasets of antimalarial â€œhitsâ€• and drugs. MedChemComm, 2010, 1, 325.	3.5	23
134	Bigger data, collaborative tools and the future of predictive drug discovery. Journal of Computer-Aided Molecular Design, 2014, 28, 997-1008.	1.3	22
135	Electron paramagnetic resonance study of isolated free radical pairs in M+18-crown-6 TCNQâ€“. (TCNQ =) Tj ETQq1 1 0.784314 rgBT /C 1991, 87, 2229-2233.	1.7	21
136	1H NMR Exchange Reactions in Tellurium(IV) Derivatives with Cleavage of Te-N Bonds. Organometallics, 1995, 14, 5258-5262.	1.1	21
137	Single-crystal electron-spin resonance study of the 4-phenyl-1,2,3,5-dithiadiazolyl radical. Magnetic Resonance in Chemistry, 1989, 27, 1161-1165.	1.1	20
138	13Câ”15N Correlation via Unsymmetrical Indirect Covariance NMR: Application to Vinblastine. Journal of Natural Products, 2007, 70, 1966-1970.	1.5	20
139	Blind trials of computer-assisted structure elucidation software. Journal of Cheminformatics, 2012, 4, 5.	2.8	20
140	Elucidating â€˜undecipherableâ€™ chemical structures using computerâ€•assisted structure elucidation approaches. Magnetic Resonance in Chemistry, 2012, 50, 22-27.	1.1	20
141	The Chemical Validation and Standardization Platform (CVSP): large-scale automated validation of chemical structure datasets. Journal of Cheminformatics, 2015, 7, 30.	2.8	20
142	Dereplication of natural products using minimal NMR data inputs. Organic and Biomolecular Chemistry, 2015, 13, 9957-9962.	1.5	20
143	High-throughput in-silico prediction of ionization equilibria for pharmacokinetic modeling. Science of the Total Environment, 2018, 615, 150-160.	3.9	19
144	¹³Câ€‹¹⁵N Connectivity networks via unsymmetrical indirect covariance processing of ¹Hâ€‹¹³C HSQC and ¹Hâ€‹¹⁵N IMPEACH spectra. Journal of Heterocyclic Chemistry, 2007, 44, 1219-1222.	1.4	18

#	Article	IF	Citations
145	Development of a Flame Retardant and an Organohalogen Flame Retardant Chemical Inventory. Scientific Data, 2022, 9, .	2.4	18
146	Application of unsymmetrical indirect covariance NMR methods to the computation of the ¹³Câ†”¹⁵N HSQCâ€ŀMPEACH and ¹³Câ†”¹⁵N HMBCâ€ŀMPEACH correlation spectra. Magnetic Resonance in Chemistry, 2007, 45, 883-888.	1.1	17
147	Why Open Drug Discovery Needs Four Simple Rules for Licensing Data and Models. PLoS Computational Biology, 2012, 8, e1002706.	1.5	17
148	Ambiguity of non-systematic chemical identifiers within and between small-molecule databases. Journal of Cheminformatics, 2015, 7, 54.	2.8	17
149	Rapid experimental measurements of physicochemical properties to inform models and testing. Science of the Total Environment, 2018, 636, 901-909.	3.9	17
150	EPR spectra of dichloro(pentamethylcyclopentadienyl)bis(trimethylphosphine)molybdenum in solution and in single crystals of (C5Me5)MoCl(PMe3)2(N2). Inorganic Chemistry, 1991, 30, 113-116.	1.9	16
151	NMR Analysis of Interfacial Structure Transitions Accompanying Electron-Transfer Threshold Transition in Reverse Microemulsions. Langmuir, 1994, 10, 4459-4467.	1.6	16
152	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. Lecture Notes in Computer Science, 2014, , 98-113.	1.0	16
153	Assessing the External Exposome Using Wearable Passive Samplers and High-Resolution Mass Spectrometry among South African Children Participating in the VHEMBE Study. Environmental Science & Technology, 2022, 56, 2191-2203.	4.6	16
154	Cosurfactant-induced electron transfer in highly resistive microemulsions. Langmuir, 1993, 9, 2782-2785.	1.6	15
155	Automated structure elucidation â€" the benefits of a symbiotic relationship between the spectroscopist and the expert system. Journal of Heterocyclic Chemistry, 2003, 40, 1017-1029.	1.4	15
156	The application of empirical methods of ¹³C NMR chemical shift prediction as a filter for determining possible relative stereochemistry. Magnetic Resonance in Chemistry, 2009, 47, 333-341.	1.1	15
157	Toward the Rational Design of Sustainable Hair Dyes Using Cheminformatics Approaches: Step 1. Database Development and Analysis. ACS Sustainable Chemistry and Engineering, 2018, 6, 2344-2352.	3.2	15
158	Carbon-13 NMR relaxation study of the overall and internal motions in compounds containingn-octyl chains. Magnetic Resonance in Chemistry, 1991, 29, 273-281.	1.1	14
159	Thermolysis of 2-benzylidenebenzocyclobutenols. Journal of Organic Chemistry, 1992, 57, 6575-6579.	1.7	14
160	Using indirect covariance spectra to identify artifact responses in unsymmetrical indirect covariance calculated spectra. Magnetic Resonance in Chemistry, 2008, 46, 138-143.	1.1	14
161	In Silico Study of In Vitro GPCR Assays by QSAR Modeling. Methods in Molecular Biology, 2016, 1425, 361-381.	0.4	14
162	Supporting non-target identification by adding hydrogen deuterium exchange MS/MS capabilities to MetFrag. Analytical and Bioanalytical Chemistry, 2019, 411, 4683-4700.	1.9	14

#	Article	IF	Citations
163	816. The oxidation of diphenylmethylenecyclobutane. Journal of the Chemical Society, 1959, , 4066.	0.4	13
164	24. Molecular polarisability. The anisotropy of the Hâ€”O bond in normal alcohols. Journal of the Chemical Society, 1960, .	0.4	13
165	Turning Spiroketals Inside Out: A Rearrangement Triggered by an Enol Ether Epoxidation. ChemistryOpen, 2015, 4, 577-580.	0.9	13
166	Connecting environmental exposure and neurodegeneration using cheminformatics and high resolution mass spectrometry: potential and challenges. Environmental Sciences: Processes and Impacts, 2019, 21, 1426-1445.	1.7	13
167	Steric effects in the system. Tetrahedron, 1965, 21, 3263-3272.	1.0	12
168	Revisiting Five Years of CASMI Contests with EPA Identification Tools. Metabolites, 2020, 10, 260.	1.3	12
169	Cheminformatics workflows using mobile apps. Chem-Bio Informatics Journal, 2013, 13, 1-18.	0.1	12
170	Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis. Analytical and Bioanalytical Chemistry, 2021, 413, 7495-7508.	1.9	12
171	363. Molecular polarisability. The molar Kerr constants of phenol and its p-methyl, chloro-, bromo-, and nitro-derivatives. Journal of the Chemical Society, 1960, .	0.4	11
172	21. The dielectric polarisations and apparent dipole moments of alcohols as solutes. Journal of the Chemical Society, 1960, .	0.4	11
173	Applications of Computer Software for the Interpretation and Management of Mass Spectrometry Data in Pharmaceutical Science. Current Topics in Medicinal Chemistry, 2002, 2, 99-107.	1.0	11
174	A new approach to automated first-order multiplet analysis. Magnetic Resonance in Chemistry, 2002, 40, 331-336.	1.1	11
175	Predicting in vivo effect levels for repeat-dose systemic toxicity using chemical, biological, kinetic and study covariates. Archives of Toxicology, 2018, 92, 587-600.	1.9	11
176	ACD/Structure Elucidator: 20 Years in the History of Development. Molecules, 2021, 26, 6623.	1.7	11
177	The evaluation of two correlation times for methyl groups from carbon-13 spin-lattice relaxation times and NOE data. Journal of Magnetic Resonance, 1990, 86, 371-375.	0.5	10
178	Singleâ€crystal electron paramagnetic resonance study of triplet excitons in [Fe(mesitylene)2+2][C3(C(CN)2)â^3]2. Journal of Chemical Physics, 1990, 93, 2222-2227.	1.2	10
179	ChemTrove: Enabling a Generic ELN To Support Chemistry through the Use of Transferable Plug-ins and Online Data Sources. Journal of Chemical Information and Modeling, 2015, 55, 501-509.	2.5	10
180	Global and internal molecular dynamics of poly(acrylamide-co-allyl) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 67 Td (2-acetamido-2-deoxy-D-g Journal of Chemistry, 1993, 71, 1995-2006.	0.6	9

#	Article	IF	Citations
181	Unsymmetrical indirect covariance processing of hyphenated and long-range heteronuclear 2D NMR spectra - Enhanced visualization of2JCHand4JCHcorrelation responses. Journal of Heterocyclic Chemistry, 2008, 45, 1109-1113.	1.4	9
182	The Future of Chemical Information Is Now. Chemistry International, 2017, 39, 9-14.	0.3	9
183	Curation of a list of chemicals in biosolids from EPA National Sewage Sludge Surveys & Biennial Review Reports. Scientific Data, 2022, 9, 180.	2.4	9
184	EPR studies of M(CO)5- radicals (M = chromium, molybdenum, tungsten) trapped in single crystals of PPN+HM(CO)5-. Organometallics, 1990, 9, 2298-2304.	1.1	8
185	EPR studies of chromium tungsten carbonyl sulfur dimer, S[M(CO)5]2-, radicals (M = chromium,) Tj ETQq1 1 0.784314 rgBT /Overloc Organometallics, 1991, 10, 180-185.	1.1	8
186	A Mechanism for Heteroatom Scrambling in the Synthesis of Unsymmetrical Chalcogenopyrylium Trimethine Dyes. Journal of Organic Chemistry, 1995, 60, 6631-6634.	1.7	8
187	Self-diffusion near the percolation threshold in reverse microemulsions. Physical Review E, 1996, 54, R5913-R5916.	0.8	8
188	ONS Open Melting Point Collection. Nature Precedings, 2011, , .	0.1	8
189	768. The polarisations and apparent dipole moments of fourteen n-alkyl bromides between methyl and octadecyl in carbon tetrachloride. Journal of the Chemical Society, 1965, .	0.4	7
190	ESR spectrum of the diiron octacarbonyl (Fe2(CO)8-) radical trapped in single crystals of bis(triphenylphosphine)nitrogen diiron octacarbonyl (PPN+HFe2(CO)8-). Organometallics, 1990, 9, 697-700.	1.1	7
191	1H and13C chemical shift assignments ofpara-substituted aryl 2-acetamido-2-deoxy-Î²-D-glucopyranosides. Magnetic Resonance in Chemistry, 1991, 29, 852-858.	1.1	7
192	Reverse micelle to sponge phase transition. Journal of Chemical Physics, 1997, 106, 7869-7872.	1.2	7
193	Automated structure elucidation of two unexpected products in a reaction of anÎ±,Î²-unsaturated pyruvate. Magnetic Resonance in Chemistry, 2004, 42, 567-572.	1.1	7
194	Multistep correlations via covariance processing of COSY/GCOSY spectra: opportunities and artifacts. Magnetic Resonance in Chemistry, 2008, 46, 997-1002.	1.1	7
195	Accessing, Using, and Creating Chemical Property Databases for Computational Toxicology Modeling. Methods in Molecular Biology, 2012, 929, 221-241.	0.4	7
196	Open Notebook Science Challenge: Solubilities of Organic Compounds in Organic Solvents. Nature Precedings, 0, , .	0.1	7
197	A harmonized chemical monitoring database for support of exposure assessments. Scientific Data, 2022, 9, .	2.4	7
198	Ageing in niobium-rich niobium-hafnium-carbon alloys. Journal of the Less Common Metals, 1970, 21, 255-273.	0.9	6

#	Article	IF	Citations
199	Electron paramagnetic resonance study of the [W(CO)4{P(OMe)3}]â"radical anion trapped in a single crystal of [N(PPh3)2][W(CO)4H{P(OMe)3}]. Journal of the Chemical Society Dalton Transactions, 1990, , 3655.	1.1	6
200	The Need for Systematic Naming Software Tools for Exchange of Chemical Information. Molecules, 1999, 4, 255-263.	1.7	6
201	A Qualitative Modeling Approach for Whole Genome Prediction Using High-Throughput Toxicogenomics Data and Pathway-Based Validation. Frontiers in Pharmacology, 2018, 9, 1072.	1.6	6
202	Alkylidenecyclobutanes. Part II. The oxidation of benzylidenecyclobutane and of bis-(p-methoxyphenyl)methylenecyclobutane. Journal of the Chemical Society C, Organic, 1966, , 655.	0.2	5
203	Spectroscopic studies. Part IX. Infrared spectra and structure of some cyclobutanecarboxylic acids. Journal of the Chemical Society B, Physical Organic, 1968, , 908.	0.2	5
204	Single-Crystal EPR Study of Triplet Excitons in Tetraethylammonium 2,3,5,6-Tetracyanobenzoquinonide. Evidence for an Interdimer Triplet Exciton. Journal of the American Chemical Society, 1995, 117, 2547-2552.	6.6	5
205	Optimization of the Ugi Reaction Using Parallel Synthesis and Automated Liquid Handling. Journal of Visualized Experiments, 2008, , .	0.2	5
206	Chemistry Crowdsourcing and Open Notebook Science. Nature Precedings, 2008, , .	0.1	5
207	InChI: connecting and navigating chemistry. Journal of Cheminformatics, 2012, 4, 33.	2.8	5
208	Using the US EPA CompTox Chemicals Dashboard to interpret targeted and non-targeted GCâ€"MS analyses from human breath and other biological media. Journal of Breath Research, 2021, 15, 025001.	1.5	5
209	Incorporating Commercial and Private Data into an Open Linked Data Platform for Drug Discovery. Lecture Notes in Computer Science, 2013, , 65-80.	1.0	5
210	325. Molecular polarisability. Chloroform as a solvent for the determination of molar Kerr constants of solutes. Journal of the Chemical Society, 1961, .	0.4	4
211	Variable-temperature high-pressure investigation of the cobalt-59 NMR spectroscopy of aqueous K3[Co(CN)6]. Magnetic Resonance in Chemistry, 2002, 40, 57-64.	1.1	4
212	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Cheminformatics, 2011, 3, .	2.8	4
213	Automated systematic nomenclature generation for organic compounds. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 150-160.	6.2	4
214	Centralized resource for chemicals from the human volatilome in an interactive open-sourced database. Journal of Breath Research, 2019, 13, 040201.	1.5	4
215	Cosurfactant facilitated transport in reverse microemulsions. , 1997, , 160-169.		4
216	Title is missing!. , 0, , .		4

#	Article	IF	Citations
217	The new alchemy: Online networking, data sharing and research activity distribution tools for scientists. F1000Research, 2017, 6, 1315.	0.8	4
218	Some enzymic syntheses of 15N-L-aspartic acid and 15N-L-glutamic acid. Canadian Journal of Chemistry, 1969, 47, 411-415.	0.6	3
219	Curing TB with open science. Tuberculosis, 2014, 94, 183-185.	0.8	3
220	Open Notebook Science Challenge: Solubilities of Organic Compounds in Organic Solvents. Nature Precedings, 0, , .	0.1	3
221	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3
222	Predicting molecular initiating events using chemical target annotations and gene expression. BioData Mining, 2022, 15, 7.	2.2	3
223	The Near Infra-Red Absorption of Normal Alcohols and their Bromides. Australian Journal of Chemistry, 1959, 12, 743.	0.5	2
224	113. Molecular polarisability: chlorobenzene as a solvent for the determination of molar Kerr constants of solutes. Journal of the Chemical Society, 1964, .	0.4	2
225	The reaction between ethyl diazoacetate and anthracene and phenanthrene. Journal of the Chemical Society C, Organic, 1969, , 68.	0.2	2
226	Electron paramagnetic resonance studies of radical pairs [M(CO) ? 5]2(M = Cr, Mo, W) trapped in single crystals of PPh + 4 HM(CO) ? 5. Journal of the Chemical Society, Faraday Transactions, 1991, 87, 3121.	1.7	2
227	Web-based information management system. TrAC - Trends in Analytical Chemistry, 1997, 16, 370-380.	5.8	2
228	Addendum to â€œUsing neural networks for 13C NMR chemical shift predictionâ€”comparison with traditional methodsâ€•[J. Magn. Reson. 157 (2002) 242â€“252]. Journal of Magnetic Resonance, 2004, 171, 1-3.	1.2	2
229	ChemSpider: How a Free Community Resource of Data Can Support the Teaching of NMR Spectroscopy. ACS Symposium Series, 2013, , 307-319.	0.5	2
230	LASSO-ing Potential Nuclear Receptor Agonists and Antagonists: A New Computational Method for Database Screening. Journal of Computational Medicine, 2013, 2013, 1-8.	0.3	2
231	25. Molecular polarisability. The molar Kerr constants at infinite dilution in benzene of seven normal alcohols. Journal of the Chemical Society, 1960, .	0.4	1
232	Alkylidenecyclobutanes. Part III. The addition of hydrogen bromide to diphenylmethylenecyclobutane. Journal of the Chemical Society C, Organic, 1969, , 390.	0.2	1
233	Beautifying Data in the Real World. Nature Precedings, 2010, , .	0.1	1
234	Chapter 12. Ligand-Based Modeling of Toxicity. RSC Drug Discovery Series, 0, , 312-344.	0.2	1

#	Article	IF	Citations
235	Utilizing open source software to facilitate communication of chemistry at RSC. , 2012, , 63-87.		1
236	Disruptive Strategies for Removing Drug Discovery Bottlenecks. Nature Precedings, 2012, , .	0.1	1
237	From chemistry to biology database curation. Drug Discovery Today: Technologies, 2015, 14, 1-2.	4.0	1
238	Reaction: How Fuzzy Are the Lines between Academia and Industry?. CheM, 2016, 1, 177-179.	5.8	1
239	ONS Open Melting Point Collection. Nature Precedings, 0, , .	0.1	1
240	Chapter 8. Covariance NMR. New Developments in NMR, 0, , 220-251.	0.1	1
241	Facilitating scientific discovery through crowdsourcing and distributed participation. EMBnet Journal, 2013, 19, 12.	0.2	1
242	ChemProt: A Disease Chemical Biology Database. , 2013, , 207-224.		1
243	Chapter 16. Small-molecule Bioactivity Databases. Chemical Biology, 2016, , 344-371.	0.1	1
244	22. Dielectric relaxation times for normal alcohols at infinite dilution in carbon tetrachloride or benzene. Journal of the Chemical Society, 1960, .	0.4	0
245	769. Molecular polarisability. The molar Kerr constants of n-alkyl bromides. Journal of the Chemical Society, 1965, .	0.4	0
246	Aerial energy surveying using infrared techniques. , 1990, , .		0
247	EPR spectra in Î³-irradiated PPN+HFeW(CO)9â¯ crystals. Magnetic Resonance in Chemistry, 1991, 29, 476-481.	1.1	0
248	Analysis of the13C and1H spectra of mixtures of benzylidene derivatives. Magnetic Resonance in Chemistry, 1994, 32, 496-498.	1.1	0
249	Substituent-induced chemical shifts of aromatic carbon centres in a series of non-acetylated and peracetylatedPara-substituted aryl 2-N-acetamido-2-deoxy-Î²-D-glucopyranosides. Magnetic Resonance in Chemistry, 1995, 33, 981-984.	1.1	0
250	Structure Elucidator: A Versatile Expert System for Molecular Structure Elucidation from 1D and 2D NMR Data and Molecular Fragments. ChemInform, 2004, 35, no.	0.1	0
251	Structure Elucidation from 2D NMR Spectra Using the StrucEluc Expert System: Detection and Removal of Contradictions in the Data.. ChemInform, 2004, 35, no.	0.1	0
252	Laboratory Information Management Systems (LIMS). , 2010, , 1255-1261.		0

#	Article	IF	Citations
253	Review of â€œContemporary computer-assisted approaches to molecular structure elucidation (new) Tj ETQq1 1 0.784314 rgBT /Ove Cheminformatics, 2013, 5, .	2.8	0
254	Turning Spiroketals Inside Out: A Rearrangement Triggered by an Enol Ether Epoxidation. ChemistryOpen, 2015, 4, 542-542.	0.9	0
255	Laboratory Information Management Systems (LIMS). , 2017, , 520-525.		0
256	Truth in structue â€“ Quicker ways to natural product structures that don't require correction. Planta Medica, 2014, 80, .	0.7	0
257	Strategies of Structure Elucidation. Lecture Notes in Quantum Chemistry II, 2015, , 53-95.	0.3	0
258	Structure Elucidation Using Strict Structure Generation. Lecture Notes in Quantum Chemistry II, 2015, , 183-306.	0.3	0
259	Fundamentals of Structure Elucidator System. Lecture Notes in Quantum Chemistry II, 2015, , 3-51.	0.3	0
260	Simple Examples of Structure Elucidation. Lecture Notes in Quantum Chemistry II, 2015, , 99-180.	0.3	0
261	Problems Solved Using Fuzzy Structure Generation. Lecture Notes in Quantum Chemistry II, 2015, , 307-444.	0.3	0
262	Increasing the reach and impact of your publications. Inform, 2016, 27, 20-23.	0.1	0