Antony John Williams

List of Publications by Citations

242 papers	9,227 citations	50 h-index	86 g-index
283 ext. papers	11,153 ext. citations	5 avg, IF	6.4 L-index

#	Paper	IF	Citations
242	ChemSpider: An Online Chemical Information Resource. *Journal of Chemical Education*, **2010**, 87, 1123-1124	2.4	629
241	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. *Journal of Cheminformatics*, **2017**, 9, 61	8.6	352
240	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, 533-54	4.2	311
239	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. *Chemical Research in Toxicology*, **2016**, 29, 1225-51	4	301
238	Comparison of different approaches to define the applicability domain of QSAR models. *Molecules*, **2012**, 17, 4791-810	4.8	276
237	Open PHACTS: semantic interoperability for drug discovery. *Drug Discovery Today*, **2012**, 17, 1188-98	8.8	229
236	In silico repositioning of approved drugs for rare and neglected diseases. *Drug Discovery Today*, **2011**, 16, 298-310	8.8	211
235	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206
234	Integrated Model of Chemical Perturbations of a Biological Pathway Using 18 In Vitro High-Throughput Screening Assays for the Estrogen Receptor. *Toxicological Sciences*, **2015**, 148, 137-54	4.4	201
233	Major structural components in freshwater dissolved organic matter. *Environmental Science & Technology*, **2007**, 41, 8240-7	10.3	175
232	OPERA models for predicting physicochemical properties and environmental fate endpoints. *Journal of Cheminformatics*, **2018**, 10, 10	8.6	151
231	Identification of "known unknowns" utilizing accurate mass data and ChemSpider. *Journal of the American Society for Mass Spectrometry*, **2012**, 23, 179-85	3.5	125
230	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. *Toxicological Sciences*, **2019**, 169, 317-332	4.4	121
229	Quantitative structure-activity relationship models for ready biodegradability of chemicals. *Journal of Chemical Information and Modeling*, **2013**, 53, 867-78	6.1	116
228	A bibliometric review of drug repurposing. *Drug Discovery Today*, **2018**, 23, 661-672	8.8	115
227	Computer-assisted structure verification and elucidation tools in NMR-based structure elucidation. *Progress in Nuclear Magnetic Resonance Spectroscopy*, **2008**, 53, 1-104	10.4	112
226	Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring. *Environment International*, **2016**, 88, 269-280	12.9	110

225	Smart Phones, a Powerful Tool in the Chemistry Classroom. *Journal of Chemical Education*, **2011**, 88, 683-686	2.4	101
224	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	6.7	98
223	Predicting hepatotoxicity using ToxCast in vitro bioactivity and chemical structure. *Chemical Research in Toxicology*, **2015**, 28, 738-51	4	96
222	A predictive ligand-based Bayesian model for human drug-induced liver injury. *Drug Metabolism and Disposition*, **2010**, 38, 2302-8	4	90
221	Towards a gold standard: regarding quality in public domain chemistry databases and approaches to improving the situation. *Drug Discovery Today*, **2012**, 17, 685-701	8.8	87
220	Exposome-Scale Investigations Guided by Global Metabolomics, Pathway Analysis, and Cognitive Computing. *Analytical Chemistry*, **2017**, 89, 11505-11513	7.8	78
219	Review of Contemporary computer-assisted approaches to molecular structure elucidation (new developments in NMR) by Mikhail E Elyashberg, Antony Williams and Kirill Blinov. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
218	The ChEMBL database as linked open data. *Journal of Cheminformatics*, **2013**, 5, 23	8.6	78
217	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, 12238-41	16.4	76
216	EPA's non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings. *Analytical and Bioanalytical Chemistry*, **2019**, 411, 853-866	4.4	73
215	Structural revisions of natural products by Computer-Assisted Structure Elucidation (CASE) systems. *Natural Product Reports*, **2010**, 27, 1296-328	15.1	71
214	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
213	Improved baseline recognition and modeling of FT NMR spectra. *Journal of Magnetic Resonance*, **2000**, 146, 122-5	3	68
212	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	5.1	68
211	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, 939-965	3.5	64
210	Internet-based tools for communication and collaboration in chemistry. *Drug Discovery Today*, **2008**, 13, 502-6	8.8	64
209	Suspect screening and non-targeted analysis of drinking water using point-of-use filters. *Environmental Pollution*, **2018**, 234, 297-306	9.3	64
208	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	6.1	63

207	Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard. *Analytical and Bioanalytical Chemistry*, **2017**, 409, 1729-1735	4.4	63
206	The use of NMR to study sodium dodecyl sulfate-gelatin interactions. *Langmuir*, **1994**, 10, 68-71	4	58
205	The application of 1H high-resolution magic-angle spinning NMR for the study of clay-organic associations in natural and synthetic complexes. *Langmuir*, **2006**, 22, 4498-503	4	56
204	Structure Elucidator: 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, 771-92		56
203	Assessing the organic composition of urban surface films using nuclear magnetic resonance spectroscopy. *Chemosphere*, **2006**, 63, 142-52	8.4	55
202	The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products. *Scientific Data*, **2018**, 5, 180125	8.2	54
201	A perspective of publicly accessible/open-access chemistry databases. *Drug Discovery Today*, **2008**, 13, 495-501	8.8	54
200	Suspect Screening Analysis of Chemicals in Consumer Products. *Environmental Science & Technology*, **2018**, 52, 3125-3135	10.3	52
199	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	7.2	52
198	EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. *Computational Toxicology*, **2019**, 12,	3.1	51
197	Computer-assisted methods for molecular structure elucidation: realizing a spectroscopist's dream. *Journal of Cheminformatics*, **2009**, 1, 3	8.6	50
196	Toward more reliable 13C and 1H chemical shift prediction: a systematic comparison of neural-network and least-squares regression based approaches. *Journal of Chemical Information and Modeling*, **2008**, 48, 128-34	6.1	50
195	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	16.4	50
194	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	2.1	48
193	Long-range carbon-carbon connectivity via unsymmetrical indirect covariance processing of HSQC and HMBC NMR data. *Magnetic Resonance in Chemistry*, **2006**, 44, 107-9	2.1	47
192	Facile Rearrangements of Alkynylamino Heterocycles with Noble Metal Cations. *Journal of Organic Chemistry*, **1996**, 61, 3289-3297	4.2	47
191	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	8.6	45
190	Identifying residues in natural organic matter through spectral prediction and pattern matching of 2D NMR datasets. *Magnetic Resonance in Chemistry*, **2004**, 42, 14-22	2.1	45

189	Identification of degradants of a complex alkaloid using NMR cryoprobe technology and ACD/structure elucidator. *Journal of Heterocyclic Chemistry*, **2002**, 39, 1241-1250	1.9	45
188	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	4.9	45
187	"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies. *Journal of Cheminformatics*, **2018**, 10, 45	8.6	44
186	NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. *Magnetic Resonance in Chemistry*, **2018**, 56, 703-715	2.1	43
185	Finding promiscuous old drugs for new uses. *Pharmaceutical Research*, **2011**, 28, 1785-91	4.5	43
184	Unsymmetrical covariance processing of COSY or TOCSY and HSQC NMR data to obtain the equivalent of HSQC-COSY or HSQC-TOCSY spectra. *Journal of Heterocyclic Chemistry*, **2006**, 43, 163-166	1.9	43
183	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	8.4	43
182	Open drug discovery for the Zika virus. *F1000Research*, **2016**, 5, 150	3.6	41
181	The Royal Society of Chemistry and the delivery of chemistry data repositories for the community. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 1023-30	4.2	40
180	Scientific competency questions as the basis for semantically enriched open pharmacological space development. *Drug Discovery Today*, **2013**, 18, 843-52	8.8	40
179	The Spectral Game: leveraging Open Data and crowdsourcing for education. *Journal of Cheminformatics*, **2009**, 1, 9	8.6	40
178	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. *Chemical Research in Toxicology*, **2021**, 34, 189-216	4	40
177	Open Science for Identifying "Known Unknown" Chemicals. *Environmental Science & Technology*, **2017**, 51, 5357-5359	10.3	39
176	Mobile apps for chemistry in the world of drug discovery. *Drug Discovery Today*, **2011**, 16, 928-39	8.8	39
175	Open-source QSAR models for pKa prediction using multiple machine learning approaches. *Journal of Cheminformatics*, **2019**, 11, 60	8.6	38
174	Using prepared mixtures of ToxCast chemicals to evaluate non-targeted analysis (NTA) method performance. *Analytical and Bioanalytical Chemistry*, **2019**, 411, 835-851	4.4	37
173	Low-Energy, Large-Angle Electron-Impact Spectra: Helium, Nitrogen, Ethylene, and Benzene. *Journal of Chemical Physics*, **1967**, 47, 4180-4185	3.9	36
172	Incorporating Green Chemistry Concepts into Mobile Chemistry Applications and Their Potential Uses. *ACS Sustainable Chemistry and Engineering*, **2013**, 1, 8-13	8.3	35

171	A comparison of three liquid chromatography (LC) retention time prediction models. *Talanta*, **2018**, 182, 371-379	6.2	34
170	Looking back to the future: predicting in vivo efficacy of small molecules versus Mycobacterium tuberculosis. *Journal of Chemical Information and Modeling*, **2014**, 54, 1070-82	6.1	34
169	When pharmaceutical companies publish large datasets: an abundance of riches or fool's gold?. *Drug Discovery Today*, **2010**, 15, 812-5	8.8	34
168	Microstructure analysis at the percolation threshold in reverse microemulsions. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **1997**, 128, 1-11	5.1	34
167	Development of a fast and accurate method of 13C NMR chemical shift prediction. *Chemometrics and Intelligent Laboratory Systems*, **2009**, 97, 91-97	3.8	33
166	Empirical and DFT GIAO quantum-mechanical methods of (13)C chemical shifts prediction: competitors or collaborators?. *Magnetic Resonance in Chemistry*, **2010**, 48, 219-29	2.1	33
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164	NMR relaxation studies of internal motions: a comparison between micelles and related systems. *The Journal of Physical Chemistry*, **1990**, 94, 2727-2729		33
163	Applying linked data approaches to pharmacology: Architectural decisions and implementation. *Semantic Web*, **2014**, 5, 101-113	2.4	32
162	An expert system for automated structure elucidation utilizing 1H-1H, 13C-1H and 15N-1H 2D NMR correlations. *Freseniusi Journal of Analytical Chemistry*, **2001**, 369, 709-14		32
161	Dispensing processes impact apparent biological activity as determined by computational and statistical analyses. *PLoS ONE*, **2013**, 8, e62325	3.7	32
160	Predicting Organ Toxicity Using in Vitro Bioactivity Data and Chemical Structure. *Chemical Research in Toxicology*, **2017**, 30, 2046-2059	4	31
159	Structure elucidation from 2D NMR spectra using the StrucEluc expert system: detection and removal of contradictions in the data. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1737-51		31
158	Analysis and elimination of artifacts in indirect covariance NMR spectra via unsymmetrical processing. *Magnetic Resonance in Chemistry*, **2005**, 43, 999-1007	2.1	31
157	Utilizing unsymmetrical indirect covariance processing to define 15N- 13C connectivity networks. *Magnetic Resonance in Chemistry*, **2007**, 45, 624-7	2.1	30
156	Automated structure verification based on a combination of 1D (1)H NMR and 2D (1)H - (13)C HSQC spectra. *Magnetic Resonance in Chemistry*, **2007**, 45, 803-13	2.1	30
155	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	2.1	30
154	The synthesis and STM/AFM imaging of 'olympicene' benzo[cd]pyrenes. *Chemistry - A European Journal*, **2015**, 21, 2011-8	4.8	28

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152	Long-Range 1H–15N Heteronuclear Shift Correlation. *Annual Reports on NMR Spectroscopy*, **2005**, 55, 1-119	1.7	28
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150	Annotating Human P-Glycoprotein Bioassay Data. *Molecular Informatics*, **2012**, 31, 599-609	3.8	27
149	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	16.4	27
148	Abstract Sifter: a comprehensive front-end system to PubMed. *F1000Research*, **2017**, 6,	3.6	27
147	Assessing bioaccumulation of polybrominated diphenyl ethers for aquatic species by QSAR modeling. *Chemosphere*, **2012**, 89, 433-44	8.4	26
146	Automated structure verification based on 1H NMR prediction. *Magnetic Resonance in Chemistry*, **2006**, 44, 524-38	2.1	26
145	Are deterministic expert systems for computer-assisted structure elucidation obsolete?. *Journal of Chemical Information and Modeling*, **2006**, 46, 1643-56	6.1	26
144	Four disruptive strategies for removing drug discovery bottlenecks. *Drug Discovery Today*, **2013**, 18, 265-8	7.8	25
143	Redefining Cheminformatics with Intuitive Collaborative Mobile Apps. *Molecular Informatics*, **2012**, 31, 569-584	3.8	24
142	Automatic vs. manual curation of a multi-source chemical dictionary: the impact on text mining. *Journal of Cheminformatics*, **2010**, 2, 3	8.6	24
141	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
140	Isolated free-radical pairs in Rb+ 18-crown-6 TCNQ− single crystals (TCNQ = tetracyanoquinodimethane). *Journal of the Chemical Society Chemical Communications*, **1990**, 439		24
139	Low-Energy Electron-Impact Study of the 12–14-eV Transitions in Nitrogen. *Journal of Chemical Physics*, **1969**, 51, 2859-2865	3.9	24
138	Prediction of Estrogenic Bioactivity of Environmental Chemical Metabolites. *Chemical Research in Toxicology*, **2016**, 29, 1410-27	4	24
137	Weaver's historic accessible collection of synthetic dyes: a cheminformatics analysis. *Chemical Science*, **2017**, 8, 4334-4339	9.4	23
136	Programmatic conversion of crystal structures into 3D printable files using Jmol. *Journal of Cheminformatics*, **2016**, 8, 66	8.6	23

135	Meta-analysis of molecular property patterns and filtering of public datasets of antimalarial Bits and drugs. *MedChemComm*, **2010**, 1, 325	5	22
134	Applying computer-assisted structure elucidation algorithms for the purpose of structure validation: revisiting the NMR assignments of hexacyclinol. *Journal of Natural Products*, **2008**, 71, 581-8	4.9	22
133	Using unsymmetrical indirect covariance processing to calculate GHSQC-COSY spectra. *Journal of Natural Products*, **2007**, 70, 1393-6	4.9	22
132	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. *Future Medicinal Chemistry*, **2015**, 7, 1921-36	4.1	21
131	Challenges and recommendations for obtaining chemical structures of industry-provided repurposing candidates. *Drug Discovery Today*, **2013**, 18, 58-70	8.8	21
130	Structure revision of asperjinone using computer-assisted structure elucidation methods. *Journal of Natural Products*, **2013**, 76, 113-6	4.9	21
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128	Parallel worlds of public and commercial bioactive chemistry data. *Journal of Medicinal Chemistry*, **2015**, 58, 2068-76	8.3	20
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122	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	3.6	19
121	Bigger data, collaborative tools and the future of predictive drug discovery. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 997-1008	4.2	19
120	(13)C-(15)N correlation via unsymmetrical indirect covariance NMR: application to vinblastine. *Journal of Natural Products*, **2007**, 70, 1966-70	4.9	19
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117	Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data. *Journal of Cheminformatics*, **2015**, 7, 9	8.6	18
116	Linking in silico MS/MS spectra with chemistry data to improve identification of unknowns. *Scientific Data*, **2019**, 6, 141	8.2	18
115	Blind trials of computer-assisted structure elucidation software. *Journal of Cheminformatics*, **2012**, 4, 5	8.6	18
114	The Chemical Validation and Standardization Platform (CVSP): large-scale automated validation of chemical structure datasets. *Journal of Cheminformatics*, **2015**, 7, 30	8.6	17
113	13C-15N Connectivity networks via unsymmetrical indirect covariance processing of 1H-13C HSQC and 1H-15N IMPEACH spectra. *Journal of Heterocyclic Chemistry*, **2007**, 44, 1219-1222	1.9	17
112	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. *Toxicology*, **2021**, 457, 152789	4.4	17
111	Elucidating 'undecipherable' chemical structures using computer-assisted structure elucidation approaches. *Magnetic Resonance in Chemistry*, **2012**, 50, 22-7	2.1	16
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109	Predictive Structure-Based Toxicology Approaches To Assess the Androgenic Potential of Chemicals. *Journal of Chemical Information and Modeling*, **2017**, 57, 2874-2884	6.1	15
108	Dereplication of natural products using minimal NMR data inputs. *Organic and Biomolecular Chemistry*, **2015**, 13, 9957-62	3.9	15
107	High-throughput in-silico prediction of ionization equilibria for pharmacokinetic modeling. *Science of the Total Environment*, **2018**, 615, 150-160	10.2	15
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103	ComputerBased Structure Elucidation from Spectral Data. *Lecture Notes in Quantum Chemistry II*, **2015**,	0.6	14
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101	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	5.1	14
100	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	12.9	13

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87	Cheminformatics workflows using mobile apps. *Chem-Bio Informatics Journal*, **2013**, 13, 1-18	0.8	11
86	Rapid experimental measurements of physicochemical properties to inform models and testing. *Science of the Total Environment*, **2018**, 636, 901-909	10.2	11
85	Development and Application of Liquid Chromatographic Retention Time Indices in HRMS-Based Suspect and Nontarget Screening. *Analytical Chemistry*, **2021**, 93, 11601-11611	7.8	11
84	In Silico Study of In Vitro GPCR Assays by QSAR Modeling. *Methods in Molecular Biology*, **2016**, 1425, 361-84		10
83	Turning Spiroketals Inside Out: A Rearrangement Triggered by an Enol Ether Epoxidation. *ChemistryOpen*, **2015**, 4, 577-80	2.3	10
82	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*, **2012**, 124, 12404-12407	3.6	10

81	Automated structure elucidation The benefits of a symbiotic relationship between the spectroscopist and the expert system. *Journal of Heterocyclic Chemistry*, **2003**, 40, 1017-1029	1.9	10
80	Carbon-13 NMR relaxation study of the overall and internal motions in compounds containing n-octyl chains. *Magnetic Resonance in Chemistry*, **1991**, 29, 273-281	2.1	10
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