Antony John Williams

List of Publications by Year in Descending Order

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	Predicting molecular initiating events using chemical target annotations and gene expression.. *BioData Mining*, **2022**, 15, 7	4.3	1
241	Curation of a list of chemicals in biosolids from EPA National Sewage Sludge Surveys & Biennial Review Reports.. *Scientific Data*, **2022**, 9, 180	8.2	0
240	Systematic Evidence Map for Over One Hundred and Fifty Per- and Polyfluoroalkyl Substances (PFAS).. *Environmental Health Perspectives*, **2022**, 130, 56001	8.4	5
239	ELIXIR and Toxicology: a community in development. *F1000Research*, **2021**, 10, 1129	3.6	0
238	Predicting compound amenability with liquid chromatography-mass spectrometry to improve non-targeted analysis. *Analytical and Bioanalytical Chemistry*, **2021**, 413, 7495-7508	4.4	3
237	Using the U.S. EPA CompTox Chemicals Dashboard to interpret targeted and non-targeted GC-MS analyses from human breath and other biological media. *Journal of Breath Research*, **2021**,	3.1	2
236	FluoroMatch 2.0-making automated and comprehensive non-targeted PFAS annotation a reality. *Analytical and Bioanalytical Chemistry*, **2021**, 1	4.4	3
235	Bioactivity profiling of per- and polyfluoroalkyl substances (PFAS) identifies potential toxicity pathways related to molecular structure. *Toxicology*, **2021**, 457, 152789	4.4	17
234	The Tox21 10K Compound Library: Collaborative Chemistry Advancing Toxicology. *Chemical Research in Toxicology*, **2021**, 34, 189-216	4	40
233	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
232	Chemical Characterization of Recycled Consumer Products Using Suspect Screening Analysis. *Environmental Science & Technology*, **2021**, 55, 11375-11387	10.3	3
231	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
230	Progress towards an OECD reporting framework for transcriptomics and metabolomics in regulatory toxicology. *Regulatory Toxicology and Pharmacology*, **2021**, 125, 105020	3.4	6
229	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	6.1	13
228	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. *Environmental Health Perspectives*, **2020**, 128, 27002	8.4	70
227	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	4.4	20
226	Revisiting Five Years of CASMI Contests with EPA Identification Tools. *Metabolites*, **2020**, 10,	5.6	8

225	Open-source QSAR models for pKa prediction using multiple machine learning approaches. *Journal of Cheminformatics*, **2019**, 11, 60	8.6	38
224	Supporting non-target identification by adding hydrogen deuterium exchange MS/MS capabilities to MetFrag. *Analytical and Bioanalytical Chemistry*, **2019**, 411, 4683-4700	4.4	9
223	The Next Generation Blueprint of Computational Toxicology at the U.S. Environmental Protection Agency. *Toxicological Sciences*, **2019**, 169, 317-332	4.4	121
222	Linking in silico MS/MS spectra with chemistry data to improve identification of unknowns. *Scientific Data*, **2019**, 6, 141	8.2	18
221	Connecting environmental exposure and neurodegeneration using cheminformatics and high resolution mass spectrometry: potential and challenges. *Environmental Sciences: Processes and Impacts*, **2019**, 21, 1426-1445	4.3	4
220	EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. *Computational Toxicology*, **2019**, 12,	3.1	51
219	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
218	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
217	EPA's non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings. *Analytical and Bioanalytical Chemistry*, **2019**, 411, 853-866	4.4	73
216	NMReDATA, a standard to report the NMR assignment and parameters of organic compounds. *Magnetic Resonance in Chemistry*, **2018**, 56, 703-715	2.1	43
215	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
214	A comparison of three liquid chromatography (LC) retention time prediction models. *Talanta*, **2018**, 182, 371-379	6.2	34
213	Suspect Screening Analysis of Chemicals in Consumer Products. *Environmental Science & Technology*, **2018**, 52, 3125-3135	10.3	52
212	Computational Tools for ADMET Profiling **2018**, 211-244		1
211	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	8.3	11
210	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
209	A bibliometric review of drug repurposing. *Drug Discovery Today*, **2018**, 23, 661-672	8.8	115
208	OPERA models for predicting physicochemical properties and environmental fate endpoints. *Journal of Cheminformatics*, **2018**, 10, 10	8.6	151

207	High-throughput in-silico prediction of ionization equilibria for pharmacokinetic modeling. *Science of the Total Environment*, **2018**, 615, 150-160	10.2	15
206	The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products. *Scientific Data*, **2018**, 5, 180125	8.2	54
205	Suspect screening and non-targeted analysis of drinking water using point-of-use filters. *Environmental Pollution*, **2018**, 234, 297-306	9.3	64
204	Predicting in vivo effect levels for repeat-dose systemic toxicity using chemical, biological, kinetic and study covariates. *Archives of Toxicology*, **2018**, 92, 587-600	5.8	7
203	A Qualitative Modeling Approach for Whole Genome Prediction Using High-Throughput Toxicogenomics Data and Pathway-Based Validation. *Frontiers in Pharmacology*, **2018**, 9, 1072	5.6	4
202	"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies. *Journal of Cheminformatics*, **2018**, 10, 45	8.6	44
201	Rapid experimental measurements of physicochemical properties to inform models and testing. *Science of the Total Environment*, **2018**, 636, 901-909	10.2	11
200	Open Science for Identifying "Known Unknown" Chemicals. *Environmental Science & Technology*, **2017**, 51, 5357-5359	10.3	39
199	Weaver's historic accessible collection of synthetic dyes: a cheminformatics analysis. *Chemical Science*, **2017**, 8, 4334-4339	9.4	23
198	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
197	Laboratory Information Management Systems (LIMS) **2017**, 520-525		
196	Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard. *Analytical and Bioanalytical Chemistry*, **2017**, 409, 1729-1735	4.4	63
195	Exposome-Scale Investigations Guided by Global Metabolomics, Pathway Analysis, and Cognitive Computing. *Analytical Chemistry*, **2017**, 89, 11505-11513	7.8	78
194	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
193	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. *Journal of Cheminformatics*, **2017**, 9, 61	8.6	352
192	Predicting Organ Toxicity Using in Vitro Bioactivity Data and Chemical Structure. *Chemical Research in Toxicology*, **2017**, 30, 2046-2059	4	31
191	The Future of Chemical Information Is Now. *Chemistry International*, **2017**, 39, 9-14	1.6	4
190	The new alchemy: Online networking, data sharing and research activity distribution tools for scientists. *F1000Research*, **2017**, 6, 1315	3.6	2

189	Abstract Sifter: a comprehensive front-end system to PubMed. *F1000Research*, **2017**, 6,	3.6	27
188	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
187	Mobile Apps for Green Chemistry **2016**, 1-9		1
186	Programmatic conversion of crystal structures into 3D printable files using Jmol. *Journal of Cheminformatics*, **2016**, 8, 66	8.6	23
185	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
184	In Silico Study of In Vitro GPCR Assays by QSAR Modeling. *Methods in Molecular Biology*, **2016**, 1425, 361-81		10
183	Big Data and Chemical Education. *Journal of Chemical Education*, **2016**, 93, 504-508	2.4	20
182	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
181	CERAPP: Collaborative Estrogen Receptor Activity Prediction Project. *Environmental Health Perspectives*, **2016**, 124, 1023-33	8.4	206
180	Open drug discovery for the Zika virus. *F1000Research*, **2016**, 5, 150	3.6	41
179	ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology. *Chemical Research in Toxicology*, **2016**, 29, 1225-51	4	301
178	Prediction of Estrogenic Bioactivity of Environmental Chemical Metabolites. *Chemical Research in Toxicology*, **2016**, 29, 1410-27	4	24
177	The synthesis and STM/AFM imaging of 'olympicene' benzo[cd]pyrenes. *Chemistry - A European Journal*, **2015**, 21, 2011-8	4.8	28
176	ComputerBased Structure Elucidation from Spectral Data. *Lecture Notes in Quantum Chemistry II*, **2015**,	0.6	14
175	Predicting hepatotoxicity using ToxCast in vitro bioactivity and chemical structure. *Chemical Research in Toxicology*, **2015**, 28, 738-51	4	96
174	Machines first, humans second: on the importance of algorithmic interpretation of open chemistry data. *Journal of Cheminformatics*, **2015**, 7, 9	8.6	18
173	Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data. *Future Medicinal Chemistry*, **2015**, 7, 1921-36	4.1	21
172	Dereplication of natural products using minimal NMR data inputs. *Organic and Biomolecular Chemistry*, **2015**, 13, 9957-62	3.9	15

171	Parallel worlds of public and commercial bioactive chemistry data. *Journal of Medicinal Chemistry*, **2015**, 58, 2068-76	8.3	20
170	Turning Spiroketals Inside Out: A Rearrangement Triggered by an Enol Ether Epoxidation. *ChemistryOpen*, **2015**, 4, 577-80	2.3	10
169	Turning Spiroketals Inside Out: A Rearrangement Triggered by an Enol Ether Epoxidation. *ChemistryOpen*, **2015**, 4, 542	2.3	
168	The Chemical Validation and Standardization Platform (CVSP): large-scale automated validation of chemical structure datasets. *Journal of Cheminformatics*, **2015**, 7, 30	8.6	17
167	Ambiguity of non-systematic chemical identifiers within and between small-molecule databases. *Journal of Cheminformatics*, **2015**, 7, 54	8.6	9
166	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
165	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, 501-9	6.1	8
164	Strategies of Structure Elucidation. *Lecture Notes in Quantum Chemistry II*, **2015**, 53-95	0.6	
163	Structure Elucidation Using Strict Structure Generation. *Lecture Notes in Quantum Chemistry II*, **2015** , 183-306	0.6	
162	Fundamentals of Structure Elucidator System. *Lecture Notes in Quantum Chemistry II*, **2015**, 3-51	0.6	
161	Simple Examples of Structure Elucidation. *Lecture Notes in Quantum Chemistry II*, **2015**, 99-180	0.6	
160	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
159	Bigger data, collaborative tools and the future of predictive drug discovery. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 997-1008	4.2	19
158	Applying linked data approaches to pharmacology: Architectural decisions and implementation. *Semantic Web*, **2014**, 5, 101-113	2.4	32
157	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
156	Curing TB with open science. *Tuberculosis*, **2014**, 94, 183-5	2.6	3
155	Scientific Lenses to Support Multiple Views over Linked Chemistry Data. *Lecture Notes in Computer Science*, **2014**, 98-113	0.9	12
154	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

153	The ChEMBL database as linked open data. *Journal of Cheminformatics*, **2013**, 5, 23	8.6	78
152	Incorporating Green Chemistry Concepts into Mobile Chemistry Applications and Their Potential Uses. *ACS Sustainable Chemistry and Engineering*, **2013**, 1, 8-13	8.3	35
151	Challenges and recommendations for obtaining chemical structures of industry-provided repurposing candidates. *Drug Discovery Today*, **2013**, 18, 58-70	8.8	21
150	Automated systematic nomenclature generation for organic compounds. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2013**, 3, 150-160	7.9	4
149	ChemSpider: How a Free Community Resource of Data Can Support the Teaching of NMR Spectroscopy. *ACS Symposium Series*, **2013**, 307-319	0.4	1
148	Quantitative structure-activity relationship models for ready biodegradability of chemicals. *Journal of Chemical Information and Modeling*, **2013**, 53, 867-78	6.1	116
147	Four disruptive strategies for removing drug discovery bottlenecks. *Drug Discovery Today*, **2013**, 18, 265-8	7.8	25
146	Scientific competency questions as the basis for semantically enriched open pharmacological space development. *Drug Discovery Today*, **2013**, 18, 843-52	8.8	40
145	Structure revision of asperjinone using computer-assisted structure elucidation methods. *Journal of Natural Products*, **2013**, 76, 113-6	4.9	21
144	LASSO-ing Potential Nuclear Receptor Agonists and Antagonists: A New Computational Method for Database Screening. *Journal of Computational Medicine*, **2013**, 2013, 1-8		2
143	Cheminformatics workflows using mobile apps. *Chem-Bio Informatics Journal*, **2013**, 13, 1-18	0.8	11
142	Dispensing processes impact apparent biological activity as determined by computational and statistical analyses. *PLoS ONE*, **2013**, 8, e62325	3.7	32
141	Incorporating Commercial and Private Data into an Open Linked Data Platform for Drug Discovery. *Lecture Notes in Computer Science*, **2013**, 65-80	0.9	5
140	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
139	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
138	Utilizing open source software to facilitate communication of chemistry at RSC **2012**, 63-87		1
137	Comparison of different approaches to define the applicability domain of QSAR models. *Molecules*, **2012**, 17, 4791-810	4.8	276
136	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

135	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
134	Assessing bioaccumulation of polybrominated diphenyl ethers for aquatic species by QSAR modeling. *Chemosphere*, **2012**, 89, 433-44	8.4	26
133	Open Drug Discovery Teams: A Chemistry Mobile App for Collaboration. *Molecular Informatics*, **2012**, 31, 585-597	3.8	28
132	Annotating Human P-Glycoprotein Bioassay Data. *Molecular Informatics*, **2012**, 31, 599-609	3.8	27
131	InChI: connecting and navigating chemistry. *Journal of Cheminformatics*, **2012**, 4, 33	8.6	5
130	Blind trials of computer-assisted structure elucidation software. *Journal of Cheminformatics*, **2012**, 4, 5	8.6	18
129	Open PHACTS: semantic interoperability for drug discovery. *Drug Discovery Today*, **2012**, 17, 1188-98	8.8	229
128	Redefining Cheminformatics with Intuitive Collaborative Mobile Apps. *Molecular Informatics*, **2012**, 31, 569-584	3.8	24
127	Elucidating 'undecipherable' chemical structures using computer-assisted structure elucidation approaches. *Magnetic Resonance in Chemistry*, **2012**, 50, 22-7	2.1	16
126	Why open drug discovery needs four simple rules for licensing data and models. *PLoS Computational Biology*, **2012**, 8, e1002706	5	15
125	Accessing, using, and creating chemical property databases for computational toxicology modeling. *Methods in Molecular Biology*, **2012**, 929, 221-41	1.4	7
124	Smart Phones, a Powerful Tool in the Chemistry Classroom. *Journal of Chemical Education*, **2011**, 88, 683-686	2.4	101
123	ONS Open Melting Point Collection. *Nature Precedings*, **2011**,		6
122	In silico repositioning of approved drugs for rare and neglected diseases. *Drug Discovery Today*, **2011**, 16, 298-310	8.8	211
121	Mobile apps for chemistry in the world of drug discovery. *Drug Discovery Today*, **2011**, 16, 928-39	8.8	39
120	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
119	Finding promiscuous old drugs for new uses. *Pharmaceutical Research*, **2011**, 28, 1785-91	4.5	43
118	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. *Journal of Cheminformatics*, **2011**, 3,	8.6	3

117	**2011**,		13
116	Laboratory Information Management Systems (LIMS) **2010**, 1255-1261		
115	A predictive ligand-based Bayesian model for human drug-induced liver injury. *Drug Metabolism and Disposition*, **2010**, 38, 2302-8	4	90
114	ChemSpider: An Online Chemical Information Resource. *Journal of Chemical Education*, **2010**, 87, 1123-11	1.24	629
113	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
112	Meta-analysis of molecular property patterns and filtering of public datasets of antimalarial hits and drugs. *MedChemComm*, **2010**, 1, 325	5	22
111	Structural revisions of natural products by Computer-Assisted Structure Elucidation (CASE) systems. *Natural Product Reports*, **2010**, 27, 1296-328	15.1	71
110	When pharmaceutical companies publish large datasets: an abundance of riches or fool's gold?. *Drug Discovery Today*, **2010**, 15, 812-5	8.8	34
109	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
108	Automatic vs. manual curation of a multi-source chemical dictionary: the impact on text mining. *Journal of Cheminformatics*, **2010**, 2, 3	8.6	24
107	. *ACS Symposium Series*, **2010**,	0.4	3
106	The application of empirical methods of (13)C NMR chemical shift prediction as a filter for determining possible relative stereochemistry. *Magnetic Resonance in Chemistry*, **2009**, 47, 333-41	2.1	11
105	A systematic approach for the generation and verification of structural hypotheses. *Magnetic Resonance in Chemistry*, **2009**, 47, 371-89	2.1	20
104	Computer-assisted methods for molecular structure elucidation: realizing a spectroscopist's dream. *Journal of Cheminformatics*, **2009**, 1, 3	8.6	50
103	The Spectral Game: leveraging Open Data and crowdsourcing for education. *Journal of Cheminformatics*, **2009**, 1, 9	8.6	40
102	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
101	Internet-based tools for communication and collaboration in chemistry. *Drug Discovery Today*, **2008**, 13, 502-6	8.8	64
100	A perspective of publicly accessible/open-access chemistry databases. *Drug Discovery Today*, **2008**, 13, 495-501	8.8	54

99	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
98	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
97	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
96	Optimization of the Ugi reaction using parallel synthesis and automated liquid handling. *Journal of Visualized Experiments*, **2008**,	1.6	3
95	Chemistry Crowdsourcing and Open Notebook Science. *Nature Precedings*, **2008**,		3
94	Using indirect covariance spectra to identify artifact responses in unsymmetrical indirect covariance calculated spectra. *Magnetic Resonance in Chemistry*, **2008**, 46, 138-43	2.1	14
93	Multistep correlations via covariance processing of COSY/GCOSY spectra: opportunities and artifacts. *Magnetic Resonance in Chemistry*, **2008**, 46, 997-1002	2.1	6
92	Unsymmetrical indirect covariance processing of hyphenated and long-range heteronuclear 2D NMR spectra - Enhanced visualization of 2JCH and 4JCH correlation responses. *Journal of Heterocyclic Chemistry*, **2008**, 45, 1109-1113	1.9	8
91	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
90	(13)C-(15)N correlation via unsymmetrical indirect covariance NMR: application to vinblastine. *Journal of Natural Products*, **2007**, 70, 1966-70	4.9	19
89	Using unsymmetrical indirect covariance processing to calculate GHSQC-COSY spectra. *Journal of Natural Products*, **2007**, 70, 1393-6	4.9	22
88	Major structural components in freshwater dissolved organic matter. *Environmental Science & Technology*, **2007**, 41, 8240-7	10.3	175
87	Fuzzy structure generation: a new efficient tool for Computer-Aided Structure Elucidation (CASE). *Journal of Chemical Information and Modeling*, **2007**, 47, 1053-66	6.1	21
86	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
85	The use of unsymmetrical indirect covariance NMR methods to obtain the equivalent of HSQC-NOESY data. *Magnetic Resonance in Chemistry*, **2007**, 45, 544-6	2.1	33
84	Utilizing unsymmetrical indirect covariance processing to define 15N- 13C connectivity networks. *Magnetic Resonance in Chemistry*, **2007**, 45, 624-7	2.1	30
83	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
82	Application of unsymmetrical indirect covariance NMR methods to the computation of the (13)C (15)N HSQC-IMPEACH and (13)C (15)N HMBC-IMPEACH correlation spectra. *Magnetic Resonance in Chemistry*, **2007**, 45, 883-8	2.1	16

81	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
80	Automated structure verification based on 1H NMR prediction. *Magnetic Resonance in Chemistry*, **2006**, 44, 524-38	2.1	26
79	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
78	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
77	Are deterministic expert systems for computer-assisted structure elucidation obsolete?. *Journal of Chemical Information and Modeling*, **2006**, 46, 1643-56	6.1	26
76	Assessing the organic composition of urban surface films using nuclear magnetic resonance spectroscopy. *Chemosphere*, **2006**, 63, 142-52	8.4	55
75	Long-Range 1H–15N Heteronuclear Shift Correlation. *Annual Reports on NMR Spectroscopy*, **2005**, 55, 1-119	1.7	28
74	Computer-aided determination of relative stereochemistry and 3D models of complex organic molecules from 2D NMR spectra. *Tetrahedron*, **2005**, 61, 9980-9989	2.4	28
73	Analysis and elimination of artifacts in indirect covariance NMR spectra via unsymmetrical processing. *Magnetic Resonance in Chemistry*, **2005**, 43, 999-1007	2.1	31
72	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
71	Automated structure elucidation of two unexpected products in a reaction of an alpha,beta-unsaturated pyruvate. *Magnetic Resonance in Chemistry*, **2004**, 42, 567-72	2.1	6
70	Addendum to "Using neural networks for 13C NMR chemical shift prediction—comparison with traditional methods" [J. Magn. Reson. 157 (2002) 242–252]. *Journal of Magnetic Resonance*, **2004**, 171, 1-3	3	2
69	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
68	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
67	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
66	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
65	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
64	A new approach to automated first-order multiplet analysis. *Magnetic Resonance in Chemistry*, **2002**, 40, 331-336	2.1	8

63	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	2.1	3
62	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
61	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	3	11
60	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
59	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
58	Improved baseline recognition and modeling of FT NMR spectra. *Journal of Magnetic Resonance*, **2000**, 146, 122-5	3	68
57	The Need for Systematic Naming Software Tools for Exchange of Chemical Information. *Molecules*, **1999**, 4, 255-263	4.8	6
56	Reverse micelle to sponge phase transition. *Journal of Chemical Physics*, **1997**, 106, 7869-7872	3.9	6
55	Microstructure analysis at the percolation threshold in reverse microemulsions. *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **1997**, 128, 1-11	5.1	34
54	Web-based information management system. *TrAC - Trends in Analytical Chemistry*, **1997**, 16, 370-380	14.6	2
53	Cosurfactant facilitated transport in reverse microemulsions **1997**, 160-169		4
52	Facile Rearrangements of Alkynylamino Heterocycles with Noble Metal Cations. *Journal of Organic Chemistry*, **1996**, 61, 3289-3297	4.2	47
51	Self-diffusion near the percolation threshold in reverse microemulsions. *Physical Review E*, **1996**, 54, R5913-R5916	2.4	8
50	A Mechanism for Heteroatom Scrambling in the Synthesis of Unsymmetrical Chalcogenopyrylium Trimethine Dyes. *Journal of Organic Chemistry*, **1995**, 60, 6631-6634	4.2	6
49	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	16.4	4
48	1H NMR Exchange Reactions in Tellurium(IV) Derivatives with Cleavage of Te-N Bonds. *Organometallics*, **1995**, 14, 5258-5262	3.8	19
47	Substituent-induced chemical shifts of aromatic carbon centres in a series of non-acetylated and peracetylated Para-substituted aryl 2-N-acetamido-2-deoxy-Ð-glucopyranosides. *Magnetic Resonance in Chemistry*, **1995**, 33, 981-984	2.1	
46	Analysis of the 13C and 1H spectra of mixtures of benzylidene derivatives. *Magnetic Resonance in Chemistry*, **1994**, 32, 496-498	2.1	

45	The use of NMR to study sodium dodecyl sulfate-gelatin interactions. *Langmuir*, **1994**, 10, 68-71	4	58
44	NMR Analysis of Interfacial Structure Transitions Accompanying Electron-Transfer Threshold Transition in Reverse Microemulsions. *Langmuir*, **1994**, 10, 4459-4467	4	15
43	Global and internal molecular dynamics of poly(acrylamide-co-allyl 2-acetamido-2-deoxy-D-glucopyranoside) glycopolymers from 13C NMR relaxation studies. *Canadian Journal of Chemistry*, **1993**, 71, 1995-2006	0.9	8
42	Cosurfactant-induced electron transfer in highly resistive microemulsions. *Langmuir*, **1993**, 9, 2782-2785	4	15
41	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	5.1	19
40	Thermolysis of 2-benzylidenebenzocyclobutenols. *Journal of Organic Chemistry*, **1992**, 57, 6575-6579	4.2	10
39	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
38	EPR spectra in □rradiated PPN+HFeW(CO)9□trystals. *Magnetic Resonance in Chemistry*, **1991**, 29, 476-481	2.1	
37	1H and 13C chemical shift assignments of para-substituted aryl 2-acetamido-2-deoxy-□D-glucopyranosides. *Magnetic Resonance in Chemistry*, **1991**, 29, 852-858	2.1	6
36	Electron paramagnetic resonance study of isolated free radical pairs in M+ 18-crown-6 TCNQ□ (TCNQ = 7,7?,8,8?-tetracyano-p-quinodimethane; M = K, Rb). *Journal of the Chemical Society, Faraday Transactions*, **1991**, 87, 2229-2233		20
35	Electron paramagnetic resonance studies of radical pairs [M(CO)□]2(M = Cr, Mo, W) trapped in single crystals of PPh+4HM(CO)□. *Journal of the Chemical Society, Faraday Transactions*, **1991**, 87, 3121		2
34	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
33	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
32	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
31	EPR studies of chromium tungsten carbonyl sulfur dimer, S[M(CO)5]2-, radicals (M = chromium, tungsten) trapped in single crystals of bis(triphenylphosphino)imium salt, PPN+HS[M(CO)5]2-. *Organometallics*, **1991**, 10, 180-185	3.8	8
30	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
29	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		9
28	Single-crystal electron paramagnetic resonance study of triplet excitons in [Fe(mesitylene)2+2][C3(C(CN)2)□]2. *Journal of Chemical Physics*, **1990**, 93, 2222-2227	3.9	6

27	NMR relaxation studies of internal motions: a comparison between micelles and related systems. *The Journal of Physical Chemistry*, **1990**, 94, 2727-2729		33
26	Electron paramagnetic resonance study of the [W(CO)4{P(OMe)3}]□ 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		6
25	Isolated free-radical pairs in Rb+ 18-crown-6 TCNQ□ single crystals (TCNQ = tetracyanoquinodimethane). *Journal of the Chemical Society Chemical Communications*, **1990**, 439		24
24	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	3.8	7
23	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	3.8	7
22	Single-crystal electron-spin resonance study of the 4-phenyl-1,2,3,5-dithiadiazolyl radical. *Magnetic Resonance in Chemistry*, **1989**, 27, 1161-1165	2.1	20
21	Ageing in niobium-rich niobium-hafnium-carbon alloys. *Journal of the Less Common Metals*, **1970**, 21, 255-273		6
20	Low-Energy Electron-Impact Study of the 12□14-eV Transitions in Nitrogen. *Journal of Chemical Physics*, **1969**, 51, 2859-2865	3.9	24
19	The reaction between ethyl diazoacetate and anthracene and phenanthrene. *Journal of the Chemical Society C, Organic*, **1969**, 68		2
18	Spectroscopic studies. Part IX. Infrared spectra and structure of some cyclobutanecarboxylic acids. *Journal of the Chemical Society B, Physical Organic*, **1968**, 908		5
17	Low-Energy, Large-Angle Electron-Impact Spectra: Helium, Nitrogen, Ethylene, and Benzene. *Journal of Chemical Physics*, **1967**, 47, 4180-4185	3.9	36
16	Alkylidenecyclobutanes. Part II. The oxidation of benzylidenecyclobutane and of bis-(p-methoxyphenyl)methylenecyclobutane. *Journal of the Chemical Society C, Organic*, **1966**, 655		5
15	Steric effects in the system. *Tetrahedron*, **1965**, 21, 3263-3272	2.4	12
14	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**, 4185-4188		7
13	113. Molecular polarisability: chlorobenzene as a solvent for the determination of molar Kerr constants of solutes. *Journal of the Chemical Society*, **1964**, 562-565		2
12	325. Molecular polarisability. Chloroform as a solvent for the determination of molar Kerr constants of solutes. *Journal of the Chemical Society*, **1961**, 1671-1676		4
11	363. Molecular polarisability. The molar Kerr constants of phenol and its p-methyl, chloro-, bromo-, and nitro-derivatives. *Journal of the Chemical Society*, **1960**, 1825-1829		11
10	24. Molecular polarisability. The anisotropy of the H□O bond in normal alcohols. *Journal of the Chemical Society*, **1960**, 123-128		12

9	21. The dielectric polarisations and apparent dipole moments of alcohols as solutes. *Journal of the Chemical Society*, **1960**, 108-115		11
8	The Near Infra-Red Absorption of Normal Alcohols and their Bromides. *Australian Journal of Chemistry*, **1959**, 12, 743	1.2	2
7	816. The oxidation of diphenylmethylenecyclobutane. *Journal of the Chemical Society*, **1959**, 4066		11
6	Chapter 12:Ligand-Based Modeling of Toxicity. *RSC Drug Discovery Series*,312-344	0.6	1
5	Structure Elucidation from 2D NMR Spectra Using the StrucEluc Expert System: Detection and Removal of Contradictions in the Data		2
4			3
3	. *Nature Precedings*,		2
2	Collaborations in Chemistry85-98		1
1	Chemspider: A Platform for Crowdsourced Collaboration to Curate Data Derived From Public Compound Databases363-386		13