David A Winkler

List of Publications by Year in Descending Order

231 papers	7,020 citations	44 h-index	74 g-index
270 ext. papers	8,381 ext. citations	7.2 avg, IF	6.5 L-index

#	Paper	IF	Citations
231	Nanoparticle-protein corona complex: understanding multiple interactions between environmental factors, corona formation, and biological activity.. *Nanotoxicology*, **2022**, 1-27	5.3	3
230	Applications of multivariate analysis and unsupervised machine learning to ToF-SIMS images of organic, bioorganic, and biological systems.. *Biointerphases*, **2022**, 17, 020802	1.8	1
229	Computational Repurposing of Drugs and Natural Products Against SARS-CoV-2 Main Protease (M) as Potential COVID-19 Therapies.. *Frontiers in Molecular Biosciences*, **2022**, 9, 781039	5.6	1
228	A bright future for engineering piezoelectric 2D crystals.. *Chemical Society Reviews*, **2021**,	58.5	3
227	Biomedical nanomaterials: applications, toxicological concerns, and regulatory needs. *Nanotoxicology*, **2021**, 15, 331-351	5.3	3
226	Use of Artificial Intelligence and Machine Learning for Discovery of Drugs for Neglected Tropical Diseases. *Frontiers in Chemistry*, **2021**, 9, 614073	5	8
225	Discovery of synergistic material-topography combinations to achieve immunomodulatory osteoinductive biomaterials using a novel in vitro screening method: The ChemoTopoChip. *Biomaterials*, **2021**, 271, 120740	15.6	9
224	In silico comparison of SARS-CoV-2 spike protein-ACE2 binding affinities across species and implications for virus origin. *Scientific Reports*, **2021**, 11, 13063	4.9	30
223	Overcoming roadblocks in computational roadmaps to the future for safe nanotechnology. *Nano Futures*, **2021**, 5, 022002	3.6	0
222	NanoSolveIT integration of tools for assessment of human and environmental exposure to nanomaterials **2021**, 81-120		0
221	Systematic Comparison of the Structural and Dynamic Properties of Commonly Used Water Models for Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2021**, 61, 4521-4536	6.1	14
220	Use of metamodels for rapid discovery of narrow bandgap oxide photocatalysts. *IScience*, **2021**, 24, 103068	6.1	4
219	Computationally repurposed drugs and natural products against RNA dependent RNA polymerase as potential COVID-19 therapies. *Molecular Biomedicine*, **2021**, 2, 28	3.1	3
218	Potent In Vitro Peptide Antagonists of the Thrombopoietin Receptor as Potential Myelofibrosis Drugs. *Advanced Therapeutics*, **2021**, 4, 2000241	4.9	
217	A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151	58.5	36
216	Exploring structure-property relationships in magnesium dissolution modulators. *Npj Materials Degradation*, **2021**, 5,	5.7	2
215	Can an InChI for Nano Address the Need for a Simplified Representation of Complex Nanomaterials across Experimental and Nanoinformatics Studies?. *Nanomaterials*, **2020**, 10,	5.4	10

214	Machine learning property prediction for organic photovoltaic devices. *Npj Computational Materials* , **2020**, 6,	10.9	20
213	Immune-Instructive Polymers Control Macrophage Phenotype and Modulate the Foreign Body Response In Vivo. *Matter*, **2020**, 2, 1564-1581	12.7	37
212	Immune Modulation by Design: Using Topography to Control Human Monocyte Attachment and Macrophage Differentiation. *Advanced Science*, **2020**, 7, 1903392	13.6	48
211	Role of Artificial Intelligence and Machine Learning in Nanosafety. *Small*, **2020**, 16, e2001883	11	33
210	Discovery of (meth)acrylate polymers that resist colonization by fungi associated with pathogenesis and biodeterioration. *Science Advances*, **2020**, 6, eaba6574	14.3	17
209	Antifibrotic strategies for medical devices. *Advanced Drug Delivery Reviews*, **2020**, 167, 109-120	18.5	14
208	NanoSolveIT Project: Driving nanoinformatics research to develop innovative and integrated tools for nanosafety assessment. *Computational and Structural Biotechnology Journal*, **2020**, 18, 583-602	6.8	41
207	Self-Organizing Map and Relational Perspective Mapping for the Accurate Visualization of High-Dimensional Hyperspectral Data. *Analytical Chemistry*, **2020**, 92, 10450-10459	7.8	16
206	QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564	58.5	196
205	Evolutionary design of optimal surface topographies for biomaterials. *Scientific Reports*, **2020**, 10, 22160	4.9	1
204	Predicting Thermal Properties of Crystals Using Machine Learning. *Advanced Theory and Simulations* , **2020**, 3, 1900208	3.5	14
203	The electronic structure of bicyclo[2.2.2]octa-2,5-dione. *Chemical Physics Letters*, **2020**, 757, 137877	2.5	
202	Ligand Entropy Is Hard but Should Not Be Ignored. *Journal of Chemical Information and Modeling*, **2020**, 60, 4421-4423	6.1	8
201	Single-Cell Tracking on Polymer Microarrays Reveals the Impact of Surface Chemistry on Twitching Speed and Biofilm Development. *ACS Applied Bio Materials*, **2020**, 3, 8471-8480	4.1	2
200	High Throughput Screening of Millions of van der Waals Heterostructures for Superlubricant Applications. *Advanced Theory and Simulations*, **2020**, 3, 2000029	3.5	4
199	Analyzing 3D hyperspectral TOF-SIMS depth profile data using self-organizing map-relational perspective mapping. *Biointerphases*, **2020**, 15, 061004	1.8	3
198	In silico screening of modulators of magnesium dissolution. *Corrosion Science*, **2020**, 163, 108245	6.8	20
197	Quantitative design rules for protein-resistant surface coatings using machine learning. *Scientific Reports*, **2019**, 9, 265	4.9	20

196	Optimal machine learning models for robust materials classification using ToF-SIMS data. *Applied Surface Science*, **2019**, 487, 773-783	6.7	17
195	Effect of mass segment size on polymer ToF-SIMS multivariate analysis using a universal data matrix. *Applied Surface Science*, **2019**, 478, 465-477	6.7	15
194	Information content of ToF-SIMS data: Effect of spectral binning. *Applied Surface Science*, **2019**, 493, 1067-1074	6.7	5
193	Coatings Releasing the Relaxin Peptide Analogue B7-33 Reduce Fibrotic Encapsulation. *ACS Applied Materials & Interfaces*, **2019**, 11, 45511-45519	9.5	6
192	Massive in Silico Study of Noble Gas Binding to the Structural Proteome. *Journal of Chemical Information and Modeling*, **2019**, 59, 4844-4854	6.1	3
191	Toward Interpretable Machine Learning Models for Materials Discovery. *Advanced Intelligent Systems*, **2019**, 1, 1900045	6	14
190	Rapid evaluation of immobilized immunoglobulins using automated mass-segmented ToF-SIMS. *Biointerphases*, **2019**, 14, 061002	1.8	3
189	Hydration and Dynamics of Ligands Determine the Antifouling Capacity of Functionalized Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 30360-30372	3.8	9
188	Evolving embodied intelligence from materials to machines. *Nature Machine Intelligence*, **2019**, 1, 12-19	22.5	47
187	Efficient Prediction of Structural and Electronic Properties of Hybrid 2D Materials Using Complementary DFT and Machine Learning Approaches. *Advanced Theory and Simulations*, **2019**, 2, 1800128	3.5	34
186	Applications in Materials Science **2018**, 547-569		1
185	Long-term dataset on aquatic responses to concurrent climate change and recovery from acidification. *Scientific Data*, **2018**, 5, 180059	8.2	5
184	Sparse QSAR modelling methods for therapeutic and regenerative medicine. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 497-509	4.2	11
183	Decoding the Rich Biological Properties of Noble Gases: How Well Can We Predict Noble Gas Binding to Diverse Proteins?. *ChemMedChem*, **2018**, 13, 1931-1938	3.7	3
182	Multivariate analysis of ToF-SIMS data using mass segmented peak lists. *Surface and Interface Analysis*, **2018**, 50, 713-728	1.5	17
181	Prediction of Broad-Spectrum Pathogen Attachment to Coating Materials for Biomedical Devices. *ACS Applied Materials & Interfaces*, **2018**, 10, 139-149	9.5	30
180	Distinguishing Chemically Similar Polyamide Materials with ToF-SIMS Using Self-Organizing Maps and a Universal Data Matrix. *Analytical Chemistry*, **2018**, 90, 12475-12484	7.8	15
179	High-Throughput Assessment and Modeling of a Polymer Library Regulating Human Dental Pulp-Derived Stem Cell Behavior. *ACS Applied Materials & Interfaces*, **2018**, 10, 38739-38748	9.5	13

178	Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. *Chemistry of Materials*, **2017**, 29, 2844-2854	9.6	123
177	Computational Approaches **2017**, 83-102		
176	Competitive Inhibition Mechanism of Acetylcholinesterase without Catalytic Active Site Interaction: Study on Functionalized C Nanoparticles via in Vitro and in Silico Assays. *ACS Applied Materials & Interfaces*, **2017**, 9, 18626-18638	9.5	29
175	Computational Modeling and Simulation of CO Capture by Aqueous Amines. *Chemical Reviews*, **2017**, 117, 9524-9593	68.1	86
174	Toward a systematic exploration of nano-bio interactions. *Toxicology and Applied Pharmacology*, **2017**, 323, 66-73	4.6	37
173	Predicting the Performance of Organic Corrosion Inhibitors. *Metals*, **2017**, 7, 553	2.3	29
172	Correction to Competitive Inhibition Mechanism of Acetylcholinesterase without Catalytic Active Site Interaction: Study on Functionalized C Nanoparticles via in Vitro and in Silico Assays. *ACS Applied Materials & Interfaces*, **2017**, 9, 44954	9.5	
171	Performance of Deep and Shallow Neural Networks, the Universal Approximation Theorem, Activity Cliffs, and QSAR. *Molecular Informatics*, **2017**, 36, 1600118	3.8	44
170	Biomimetic molecular design tools that learn, evolve, and adapt. *Beilstein Journal of Organic Chemistry*, **2017**, 13, 1288-1302	2.5	5
169	Computational Modelling of Magnetic Nanoparticle Properties and In Vivo Responses. *Current Medicinal Chemistry*, **2017**, 24, 483-496	4.3	8
168	A thrombopoietin receptor antagonist is capable of depleting myelofibrosis hematopoietic stem and progenitor cells. *Blood*, **2016**, 127, 3398-409	2.2	19
167	Aluminum toxicity risk reduction as a result of reduced acid deposition in Adirondack lakes and ponds. *Environmental Monitoring and Assessment*, **2016**, 188, 636	3.1	4
166	A renaissance of neural networks in drug discovery. *Expert Opinion on Drug Discovery*, **2016**, 11, 785-95	6.2	127
165	Understanding the Roles of the "Two QSARs". *Journal of Chemical Information and Modeling*, **2016**, 56, 269-74	6.1	95
164	Accurate and interpretable nanoSAR models from genetic programming-based decision tree construction approaches. *Nanotoxicology*, **2016**, 10, 1001-12	5.3	26
163	Using high throughput experimental data and in silico models to discover alternatives to toxic chromate corrosion inhibitors. *Corrosion Science*, **2016**, 106, 229-235	6.8	68
162	The diverse biological properties of the chemically inert noble gases. *Pharmacology & Therapeutics*, **2016**, 160, 44-64	13.9	31
161	Modeling the Influence of Fatty Acid Incorporation on Mesophase Formation in Amphiphilic Therapeutic Delivery Systems. *Molecular Pharmaceutics*, **2016**, 13, 996-1003	5.6	8

160	Recent advances, and unresolved issues, in the application of computational modelling to the prediction of the biological effects of nanomaterials. *Toxicology and Applied Pharmacology*, **2016**, 299, 96-100	4.6	55
159	Validating Eaton's Hypothesis: Cubane as a Benzene Bioisostere. *Angewandte Chemie*, **2016**, 128, 3644-3649	3.8	28
158	An Experimental and Computational Approach to the Development of ZnO Nanoparticles that are Safe by Design. *Small*, **2016**, 12, 3568-77	11	47
157	Validating Eaton's Hypothesis: Cubane as a Benzene Bioisostere. *Angewandte Chemie - International Edition*, **2016**, 55, 3580-5	16.4	78
156	Frontispiece: Validating Eaton's Hypothesis: Cubane as a Benzene Bioisostere. *Angewandte Chemie - International Edition*, **2016**, 55,	16.4	1
155	Glossary of terms used in computational drug design, part II (IUPAC Recommendations 2015). *Pure and Applied Chemistry*, **2016**, 88, 239-264	2.1	8
154	Discovery and Optimization of Materials Using Evolutionary Approaches. *Chemical Reviews*, **2016**, 116, 6107-32	68.1	107
153	Molecular Markers for Pyrethrin Autoxidation in Stored Pyrethrum Crop: Analysis and Structure Determination. *Journal of Agricultural and Food Chemistry*, **2016**, 64, 7134-41	5.7	5
152	Relevance Vector Machines: Sparse Classification Methods for QSAR. *Journal of Chemical Information and Modeling*, **2015**, 55, 1529-34	6.1	39
151	Beware of R(2): Simple, Unambiguous Assessment of the Prediction Accuracy of QSAR and QSPR Models. *Journal of Chemical Information and Modeling*, **2015**, 55, 1316-22	6.1	350
150	Sparse feature selection methods identify unexpected global cellular response to strontium-containing materials. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 4280-5	11.5	52
149	Towards computational design of zeolite catalysts for CO2 reduction. *RSC Advances*, **2015**, 5, 44361-44370	3.7	30
148	Thermostability and reversibility of silver nanoparticle-protein binding. *Physical Chemistry Chemical Physics*, **2015**, 17, 1728-39	3.6	26
147	Immobilisation of a thrombopoietin peptidic mimic by self-assembled monolayers for culture of CD34+ cells. *Biomaterials*, **2015**, 37, 82-93	15.6	8
146	Chemistry spacetime. *Perspectives in Science*, **2015**, 6, 2-14	0.8	4
145	Illuminating Flash Point: Comprehensive Prediction Models. *Molecular Informatics*, **2015**, 34, 18-27	3.8	4
144	Robust Prediction of Personalized Cell Recognition from a Cancer Population by a Dual Targeting Nanoparticle Library. *Advanced Functional Materials*, **2015**, 25, 6927-6935	15.6	15
143	A Bright Future for Evolutionary Methods in Drug Design. *ChemMedChem*, **2015**, 10, 1296-300	3.7	15

142	Surface-water Interface Induces Conformational Changes Critical for Protein Adsorption: Implications for Monolayer Formation of EAS Hydrophobin. *Frontiers in Molecular Biosciences*, **2015**, 2, 64	5.6	23
141	Discovery of a Novel Polymer for Human Pluripotent Stem Cell Expansion and Multilineage Differentiation. *Advanced Materials*, **2015**, 27, 4006-12	24	64
140	Adrien Albert Award: How to Mine Chemistry Space for New Drugs and Biomedical Therapies. *Australian Journal of Chemistry*, **2015**, 68, 1174	1.2	3
139	Probing enzyme-nanoparticle interactions using combinatorial gold nanoparticle libraries. *Nano Research*, **2015**, 8, 1293-1308	10	26
138	Sparse feature selection identifies H2A.Z as a novel, pattern-specific biomarker for asymmetrically self-renewing distributed stem cells. *Stem Cell Research*, **2015**, 14, 144-54	1.6	12
137	Brooktrout Lake case study: biotic recovery from acid deposition 20 years after the 1990 Clean Air Act Amendments. *Environmental Science & Technology*, **2015**, 49, 2665-74	10.3	22
136	Modelling and predicting the biological effects of nanomaterials. *SAR and QSAR in Environmental Research*, **2014**, 25, 161-72	3.5	74
135	Ultrafast Fabrication of Covalently Cross-linked Multifunctional Graphene Oxide Monoliths. *Advanced Functional Materials*, **2014**, 24, 4915-4921	15.6	86
134	Materials for stem cell factories of the future. *Nature Materials*, **2014**, 13, 570-9	27	126
133	Getting to the source: selective drug targeting of cancer stem cells. *ChemMedChem*, **2014**, 9, 885-98	3.7	8
132	Graphene Oxide: Ultrafast Fabrication of Covalently Cross-linked Multifunctional Graphene Oxide Monoliths (Adv. Funct. Mater. 31/2014). *Advanced Functional Materials*, **2014**, 24, 4914-4914	15.6	
131	Contrasting Effects of Nanoparticle Binding on Protein Denaturation. *Journal of Physical Chemistry C*, **2014**, 118, 22069-22078	3.8	28
130	Towards chromate-free corrosion inhibitors: structure–property models for organic alternatives. *Green Chemistry*, **2014**, 16, 3349-3357	10	93
129	Modelling and Prediction of Bacterial Attachment to Polymers. *Advanced Functional Materials*, **2014**, 24, 2085-2093	15.6	38
128	A Thrombopoietin Antagonist Is Capable of Affecting Stem and Progenitor Cells of Patients with Myelofibrosis. *Blood*, **2014**, 124, 819-819	2.2	
127	Potent agonists of a hematopoietic stem cell cytokine receptor, c-Mpl. *ChemMedChem*, **2013**, 8, 763-71	3.7	4
126	Capturing the crystal: prediction of enthalpy of sublimation, crystal lattice energy, and melting points of organic compounds. *Journal of Chemical Information and Modeling*, **2013**, 53, 223-9	6.1	44
125	Predicting the complex phase behavior of self-assembling drug delivery nanoparticles. *Molecular Pharmaceutics*, **2013**, 10, 1368-77	5.6	18

124	Aqueous solubility prediction: do crystal lattice interactions help?. *Molecular Pharmaceutics*, **2013**, 10, 2757-66	5.6	46
123	Predicting the Effect of Lipid Structure on Mesophase Formation during in Meso Crystallization. *Crystal Growth and Design*, **2013**, 13, 3126-3137	3.5	5
122	Applying quantitative structure-activity relationship approaches to nanotoxicology: current status and future potential. *Toxicology*, **2013**, 313, 15-23	4.4	132
121	Computational Modeling and Prediction of the Complex Time-Dependent Phase Behavior of Lyotropic Liquid Crystals under in Meso Crystallization Conditions. *Crystal Growth and Design*, **2013**, 13, 1267-1276	3.5	12
120	Mesenchymal stromal cell turnover in the normal adult lung revisited. *American Journal of Physiology - Lung Cellular and Molecular Physiology*, **2013**, 305, L635-41	5.8	3
119	Self-organizing circuitry and emergent computation in mouse embryonic stem cells. *Stem Cell Research*, **2012**, 8, 324-33	1.6	16
118	Modelling human embryoid body cell adhesion to a combinatorial library of polymer surfaces. *Journal of Materials Chemistry*, **2012**, 22, 20902-20906		37
117	Unzipping the role of chirality in nanoscale self-assembly of tripeptide hydrogels. *Nanoscale*, **2012**, 4, 6752-60	7.7	89
116	Modeling biological activities of nanoparticles. *Nano Letters*, **2012**, 12, 5808-12	11.5	148
115	Structure and Function of Ecdysone Receptors: Interactions with Ecdysteroids and Synthetic Agonists. *Advances in Insect Physiology*, **2012**, 43, 299-351	2.5	13
114	Computational Approaches **2012**, 85-96		1
113	Quantitative structure-property relationship modeling of diverse materials properties. *Chemical Reviews*, **2012**, 112, 2889-919	68.1	320
112	Robust, quantitative tools for modelling ex-vivo expansion of haematopoietic stem cells and progenitors. *Molecular BioSystems*, **2012**, 8, 913-20		8
111	Principal signalling complexes in haematopoiesis: structural aspects and mimetic discovery. *Cytokine and Growth Factor Reviews*, **2011**, 22, 231-53	17.9	8
110	Tripeptide motifs in biology: targets for peptidomimetic design. *Journal of Medicinal Chemistry*, **2011**, 54, 1111-25	8.3	51
109	A general model for binary cell fate decision gene circuits with degeneracy: indeterminacy and switch behavior in the absence of cooperativity. *PLoS ONE*, **2011**, 6, e19358	3.7	41
108	Modeling the molecular basis for 41 integrin antagonism. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 5903-11	3.4	6
107	Modelling topoisomerase I inhibition by minor groove binders. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 1450-7	3.4	6

106	Binding inhibitors of the bacterial sliding clamp by design. *Journal of Medicinal Chemistry*, **2011**, 54, 483188	5	31
105	Zinc is not required for activity of TPO agonists acting at the c-Mpl receptor transmembrane domain. *ACS Chemical Biology*, **2010**, 5, 741-5	4.9	5
104	Robust modelling of solubility in supercritical carbon dioxide using Bayesian methods. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 593-7	2.8	25
103	Modelling inhalational anaesthetics using bayesian feature selection and QSAR modelling methods. *ChemMedChem*, **2010**, 5, 1318-23	3.7	6
102	Synthesis, binding and bioactivity of gamma-methylene gamma-lactam ecdysone receptor ligands: advantages of QSAR models for flexible receptors. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 5647-60	3.4	25
101	Predictive mesoscale network model of cell fate decisions during C. elegans embryogenesis. *Artificial Life*, **2009**, 15, 411-21	1.4	5
100	Stem cell decision making and critical-like exploratory networks. *Stem Cell Research*, **2009**, 2, 165-77	1.6	16
99	Modelling atypical small-molecule mimics of an important stem cell cytokine, thrombopoietin. *ChemMedChem*, **2009**, 4, 2002-11	3.7	7
98	Optimal Sparse Descriptor Selection for QSAR Using Bayesian Methods. *QSAR and Combinatorial Science*, **2009**, 28, 645-653		56
97	An Optimal Self-Pruning Neural Network and Nonlinear Descriptor Selection in QSAR. *QSAR and Combinatorial Science*, **2009**, 28, 1092-1097		48
96	A Carbon-13 NMR Study of Carbon Dioxide Absorption and Desorption with Aqueous Amine Solutions. *Energy Procedia*, **2009**, 1, 955-962	2.3	44
95	Toward novel universal descriptors: charge fingerprints. *Journal of Chemical Information and Modeling*, **2009**, 49, 710-5	6.1	26
94	Toward a Rosetta stone for the stem cell genome: stochastic gene expression, network architecture, and external influences. *Stem Cell Research*, **2008**, 1, 157-68	1.6	10
93	Bayesian regularization of neural networks. *Methods in Molecular Biology*, **2008**, 458, 25-44	1.4	224
92	Network models in drug discovery and regenerative medicine. *Biotechnology Annual Review*, **2008**, 14, 143-70		5
91	A Methodology for Applying Energy Harvesting to Extend Wildlife Tag Lifetime **2008**,		4
90	Classification of emergence and its relation to self-organization. *Complexity*, **2008**, 13, 10-15	1.6	68
89	Consistent concepts of self-organization and self-assembly. *Complexity*, **2008**, 14, 10-17	1.6	107

88	Critical-like self-organization and natural selection: two facets of a single evolutionary process?. *BioSystems*, **2008**, 92, 148-58	1.9	26
87	Parasiticidal 2-alkoxy- and 2-aryloxyiminoalkyl trifluoromethanesulfonanilides. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 252-5	2.9	6
86	Discovery of (Z)-2-phenyl-3-(1H-pyrrol-2-yl)acrylonitrile derivatives active against Haemonchus contortus and Ctenocephalides felis (cat flea). *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 993-7	2.9	15
85	Nonlinear predictive modeling of MHC class II-peptide binding using Bayesian neural networks. *Methods in Molecular Biology*, **2007**, 409, 365-77	1.4	2
84	An experimental and theoretical study into the valence electronic structure of bicyclo[2.2.1]hepta-2,5-dione. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2006**, 39, 2411-2429	1.3	5
83	Simulation and Modelling of Chemical and Biological Complex Systems. *Australian Journal of Chemistry*, **2006**, 59, 859	1.2	4
82	Orbital based electronic structural signatures of the guanine keto G-7H/G-9H tautomer pair as studied using dual space analysis. *Biophysical Chemistry*, **2006**, 121, 105-20	3.5	26
81	Classification of Self-Organization and Emergence in Chemical and Biological Systems. *Australian Journal of Chemistry*, **2006**, 59, 849	1.2	6
80	Investigation into the valence electronic structure of norbornene using electron momentum spectroscopy, Green's function, and density functional theories. *Journal of Physical Chemistry A*, **2005**, 109, 9324-40	2.8	28
79	Predictive Bayesian neural network models of MHC class II peptide binding. *Journal of Molecular Graphics and Modelling*, **2005**, 23, 481-9	2.8	29
78	The X-ray structure of a hemipteran ecdysone receptor ligand-binding domain: comparison with a lepidopteran ecdysone receptor ligand-binding domain and implications for insecticide design. *Journal of Biological Chemistry*, **2005**, 280, 22258-69	5.4	91
77	Overview of Quantitative Structure□Activity Relationships (QSAR) **2005**, 347-367		1
76	Predictive Human Intestinal Absorption QSAR Models Using Bayesian Regularized Neural Networks. *Australian Journal of Chemistry*, **2005**, 58, 859	1.2	20
75	Neural networks as robust tools in drug lead discovery and development. *Molecular Biotechnology*, **2004**, 27, 139-68	3	67
74	Structural impact on the methano bridge in norbornadiene, norbornene and norbornane. *Journal of Physics and Chemistry of Solids*, **2004**, 65, 2041-2054	3.9	8
73	Modelling blood-brain barrier partitioning using Bayesian neural nets. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 499-505	2.8	56
72	Broad-based quantitative structure-activity relationship modeling of potency and selectivity of farnesyltransferase inhibitors using a Bayesian regularized neural network. *Journal of Medicinal Chemistry*, **2004**, 47, 6230-8	8.3	30
71	Norbornane: an investigation into its valence electronic structure using electron momentum spectroscopy, and density functional and Green's function theories. *Journal of Chemical Physics*, **2004**, 121, 10525-41	3.9	40

70	Synthesis, Biological Activity, and QSAR Studies of Antimicrobial Agents Containing Biguanide Isosteres. *Australian Journal of Chemistry*, **2004**, 57, 77	1.2	8
69	Bayesian neural nets for modeling in drug discovery. *Drug Discovery Today Biosilico*, **2004**, 2, 104-111		21
68	Rapid prediction of chemical metabolism by human UDP-glucuronosyltransferase isoforms using quantum chemical descriptors derived with the electronegativity equalization method. *Journal of Medicinal Chemistry*, **2004**, 47, 5311-7	8.3	42
67	Neural networks in ADME and toxicity prediction. *Drugs of the Future*, **2004**, 29, 1043	2.3	23
66	An electron momentum spectroscopy and density functional theory study of the outer valence electronic structure of stella-2,6-dione. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2003**, 36, 3155-3171	1.3	16
65	Comparison of linear and nonlinear classification algorithms for the prediction of drug and chemical metabolism by human UDP-glucuronosyltransferase isoforms. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 2019-24		67
64	Exploring the electronic structure of 2,6-stelladione from momentum space I: the p-dominant molecular orbitals in the outer valence shell. *Chemical Physics Letters*, **2003**, 382, 217-225	2.5	16
63	Definitive confirmation for through-space bond dominance in the outermost □orbitals of norbornadiene. *Journal of Electron Spectroscopy and Related Phenomena*, **2002**, 123, 389-395	1.7	17
62	Comprehensive Experimental and Theoretical Study into the Complete Valence Electronic Structure of Norbornadiene. *Journal of Physical Chemistry A*, **2002**, 106, 9573-9581	2.8	16
61	Application of neural networks to large dataset QSAR, virtual screening, and library design. *Methods in Molecular Biology*, **2002**, 201, 325-67	1.4	10
60	The role of quantitative structure--activity relationships (QSAR) in biomolecular discovery. *Briefings in Bioinformatics*, **2002**, 3, 73-86	13.4	100
59	Core molecular orbital contribution to N2O isomerization as studied using theoretical electron momentum spectroscopy. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2001**, 57, 9-15	4.4	14
58	Structure-based design of inhibitors of the rice blast fungal enzyme trihydroxynaphthalene reductase. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 434-47, 470-1	2.8	35
57	A high-resolution electron momentum spectroscopy and density functional theory study into the complete valence electronic structure of allene. *Journal of Computational Chemistry*, **2001**, 22, 1321-1333	3.5	13
56	A Density Functional Theory and Electron Momentum Spectroscopy Study into the Complete Valence Electronic Structure of Cubane. *Journal of the American Chemical Society*, **2000**, 122, 3892-3900	16.4	30
55	Robust QSAR Models from Novel Descriptors and Bayesian Regularised Neural Networks. *Molecular Simulation*, **2000**, 24, 243-258	2	50
54	A quantitative structure--activity relationships model for the acute toxicity of substituted benzenes to Tetrahymena pyriformis using Bayesian-regularized neural networks. *Chemical Research in Toxicology*, **2000**, 13, 436-40	4	82
53	Use of automatic relevance determination in QSAR studies using Bayesian neural networks. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1423-30		109

52	The Computer Simulation of High Throughput Screening of Bioactive Molecules **2000**, 175-180		1
51	New QSAR Methods Applied to Structure Activity Mapping and Combinatorial Chemistry. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 236-242		55
50	Synthesis of homorhamnojirimycins and related trihydroxypipecolic acid derivatives via divergent bicyclic amino lactone intermediates: Inhibition of naringinase (L-rhamnosidase) and dTDP-rhamnose biosynthesis. *Journal of the Chemical Society Perkin Transactions 1*, **1999**, 2735-2745		25
49	Investigation of 5-HT4 agonist activities using molecular field analysis. *Journal of the Chemical Society Perkin Transactions II*, **1999**, 153-158		5
48	Piperidine analogues of D-galactose as potent inhibitors of galactosidase: Synthesis by stannane-mediated hydroxymethylation of 5-azido-1,4-lactones. Structural relationships between D-galactosidase and L-rhamnosidase inhibitors. *Journal of the Chemical Society Perkin Transactions 1* , **1999**, 2747-2754		19
47	Robust QSAR models using Bayesian regularized neural networks. *Journal of Medicinal Chemistry*, **1999**, 42, 3183-7	8.3	204
46	An electron momentum spectroscopy and density functional theory investigation into the complete valence electronic structure of ethylene oxide. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **1999**, 32, 3239-3253	1.3	8
45	Atomistic Topological Indices Applied to Benzodiazepines using Various Regression Methods. *QSAR and Combinatorial Science*, **1998**, 17, 14-19		20
44	Holographic QSAR of Benzodiazepines. *QSAR and Combinatorial Science*, **1998**, 17, 224-231		4
43	Potential intermediates for incorporation of polyhydroxylated prolines into combinatorial libraries. *Tetrahedron Letters*, **1998**, 39, 6091-6094	2	14
42	5-epi-Deoxyrhamnojirimycin is a potent inhibitor of an -rhamnosidase: 5-epi-deoxymannojirimycin is not a potent inhibitor of an d-mannosidase. *Tetrahedron: Asymmetry*, **1998**, 9, 2947-2960		37
41	Transformation of substituted 2H-pyran-5-carboxylates into 3R*-vinyl-1,2R*-cyclopropanedicarboxylates. *New Journal of Chemistry*, **1998**, 22, 1485-1492	3.6	7
40	Momentum distributions and molecular property information for trans 1,3 butadiene: An electron momentum spectroscopy and density functional theory investigation. *Journal of Chemical Physics*, **1998**, 108, 1859-1873	3.9	13
39	Application of DFT and EMS to the Study of Strained Organic Molecules. *Australian Journal of Physics*, **1998**, 51, 707		9
38	Holographic QSAR of Benzodiazepines. *QSAR and Combinatorial Science*, **1998**, 17, 224-231		20
37	Theoretical and (e,2e) Experimental Investigation into the Complete Valence Electronic Structure of [1.1.1]Propellane. *Journal of the American Chemical Society*, **1997**, 119, 2896-2904	16.4	26
36	Predicting maximum bioactivity by effective inversion of neural networks using genetic algorithms. *Chemometrics and Intelligent Laboratory Systems*, **1997**, 38, 127-137	3.8	16
35	Molecular modeling studies of "flap up" mannosyl cation mimics. *Journal of Medicinal Chemistry*, **1996**, 39, 4332-4	8.3	31

34	The Synthesis of Bisguanidinoalkanes and Guanidinoalkanes, N- or N'-Substituted With Pyrimidines, as Analogues of Chlorhexidine. *Australian Journal of Chemistry*, **1996**, 49, 573	1.2	2
33	2-Doping of 1,4-polydienes. *Synthetic Metals*, **1995**, 69, 563-566	3.6	19
32	Electron momentum spectroscopy of [1.1.1]propellane. *Chemical Physics Letters*, **1995**, 244, 433-439	2.5	6
31	Conducting Polymers from Polybutadiene: Molecular Configuration Effects on the Iodine-Induced Conjugation Reactions. *Macromolecules*, **1994**, 27, 6728-6735	5.5	31
30	6-(2-Methylpropylthio)-2-pyridyl methanesulfonate. *Acta Crystallographica Section C: Crystal Structure Communications*, **1993**, 49, 2039-2040		
29	Preparation of Bicyclic Herbicide Precursors by Intramolecular Stork-Danheiser Kinetic Alkylation Reactions of Methyl 1-(Haloalkyl)-3-methoxy-5-oxocyclohex-3-ene-1-carboxylate Derivatives. *Australian Journal of Chemistry*, **1992**, 45, 759	1.2	2
28	Carbocation-Mediated Rearrangements Within [n.m.1]Propellane Frameworks. *Australian Journal of Chemistry*, **1991**, 44, 593	1.2	2
27	Transition-state analogues as inhibitors for GABA-aminotransferase. *European Journal of Medicinal Chemistry*, **1991**, 26, 129-135	6.8	3
26	Quantitative structure-activity studies of pyrethroids. *Pesticide Biochemistry and Physiology*, **1991**, 41, 29-40	4.9	
25	Morpheus: a conformation-activity relationships and receptor modeling package. *Journal of Molecular Graphics*, **1989**, 7, 138-45		8
24	A molecular graphics study of factors influencing herbicidal activity of oximes of 3-acyl-tetrahydro-2H-pyran-2,4-diones. *Pest Management Science*, **1989**, 27, 45-63		10
23	Design of potential anti-HIV agents. 1. Mannosidase inhibitors. *Journal of Medicinal Chemistry*, **1989**, 32, 2084-9	8.3	118
22	The non-Fickian diffusion of deterrents into a nitrocellulose-based propellant. *Journal of Applied Polymer Science*, **1988**, 35, 51-62	2.9	7
21	Molecular orbital studies of reaction mechanism and transition state structures for GABA-transaminase. *European Journal of Medicinal Chemistry*, **1988**, 23, 125-132	6.8	9
20	The conformations of 1,1,2,2-tetracyanoethane and 1,2-dichlorotetracyanoethane: a molecular orbital, dipole moment and kerr effect study. *Journal of Molecular Structure*, **1988**, 172, 291-298	3.4	3
19	Quantitative Structure-Activity Relationships in Insecticidal Pyrethroid Ethers. *QSAR and Combinatorial Science*, **1988**, 7, 79-84		2
18	Targeted cytotoxic cells as a novel form of cancer immunotherapy. *Molecular Immunology*, **1988**, 25, 1093-103	4.3	25
17	Re.: Invalidation of Lowry protein estimations and macrophage [3H]deoxyglucose uptake by plastic tubes and airflow. *Journal of Immunological Methods*, **1987**, 98, 285-6	2.5	

16	A conformational study of the topographical requirements of a phytotropin recognition site on the naphthylphthalamic acid receptor. *Phytochemistry*, **1987**, 26, 2881-2889	4	14
15	Molecular conformational studies of cellulose nitrate. *Polymer*, **1986**, 27, 765-768	3.9	4
14	Conformational energy calculations and electrostatic potentials of dihydrofolate reductase ligands: relevance to mode of binding and species specificity. *Journal of Medicinal Chemistry*, **1986**, 29, 698-708	8.3	16
13	Design, Synthesis and Testing of Transition State Analogues of Alanine Racemase as Antibacterials. *Australian Journal of Chemistry*, **1985**, 38, 297	1.2	4
12	Structure-activity relationships of convulsant and anticonvulsant barbiturates: a computer-graphic-based pattern-recognition analysis. *Journal of Medicinal Chemistry*, **1983**, 26, 1223-9	8.3	15
11	Conformational analysis of picrotoxinin by N.M.R., X-ray crystallography, and molecular orbital and classical potential-energy calculations. *Australian Journal of Chemistry*, **1983**, 36, 2219	1.2	8
10	Conformational analysis of the ergot alkaloids ergotamine and ergotaminine. *Journal of Medicinal Chemistry*, **1982**, 25, 937-42	8.3	46
9	Hyperfine interactions in methanimine. *Australian Journal of Chemistry*, **1982**, 35, 667	1.2	17
8	Hyperfine interactions in the microwave spectrum of 2-propen-1-Imine (vinylimine). *Chemical Physics*, **1981**, 59, 243-247	2.3	11
7	The microwave spectrum of HCN dimer. *Journal of Molecular Spectroscopy*, **1981**, 89, 352-355	1.3	35
6	The microwave spectrum of (Z)-Ethanimine. *Australian Journal of Chemistry*, **1980**, 33, 1	1.2	10
5	Detection of the 23-22 emission line of sulphur monoxide and its relevance to magnetic fields in Orion. *Monthly Notices of the Royal Astronomical Society*, **1980**, 190, 1-6	4.3	2
4	Detection of J = 2 -> 1 emission of acetonitrile (CH3CN) in Sgr B2. *Monthly Notices of the Royal Astronomical Society*, **1977**, 180, 1P-3P	4.3	2
3	Deep and Shallow Neural Networks453-464		1
2	Synergistic Material-Topography Combinations to Achieve Immunomodulatory Osteogenic Biomaterials		1
1	Active Learning in Bayesian Neural Networks for Bandgap Predictions of Novel Van der Waals Heterostructures. *Advanced Intelligent Systems*,2100080	6	1