# David A Winkler

## List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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|---|---|---|---|
| 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 | 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 |
| 230 | Quantitative structure-property relationship modeling of diverse materials properties. *Chemical Reviews*, **2012**, 112, 2889-919 | 68.1 | 320 |
| 229 | Bayesian regularization of neural networks. *Methods in Molecular Biology*, **2008**, 458, 25-44 | 1.4 | 224 |
| 228 | Robust QSAR models using Bayesian regularized neural networks. *Journal of Medicinal Chemistry*, **1999**, 42, 3183-7 | 8.3 | 204 |
| 227 | QSAR without borders. *Chemical Society Reviews*, **2020**, 49, 3525-3564 | 58.5 | 196 |
| 226 | Modeling biological activities of nanoparticles. *Nano Letters*, **2012**, 12, 5808-12 | 11.5 | 148 |
| 225 | Applying quantitative structure-activity relationship approaches to nanotoxicology: current status and future potential. *Toxicology*, **2013**, 313, 15-23 | 4.4 | 132 |
| 224 | A renaissance of neural networks in drug discovery. *Expert Opinion on Drug Discovery*, **2016**, 11, 785-95 | 6.2 | 127 |
| 223 | Materials for stem cell factories of the future. *Nature Materials*, **2014**, 13, 570-9 | 27 | 126 |
| 222 | Materials Genome in Action: Identifying the Performance Limits of Physical Hydrogen Storage. *Chemistry of Materials*, **2017**, 29, 2844-2854 | 9.6 | 123 |
| 221 | Design of potential anti-HIV agents. 1. Mannosidase inhibitors. *Journal of Medicinal Chemistry*, **1989**, 32, 2084-9 | 8.3 | 118 |
| 220 | Use of automatic relevance determination in QSAR studies using Bayesian neural networks. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1423-30 | | 109 |
| 219 | Consistent concepts of self-organization and self-assembly. *Complexity*, **2008**, 14, 10-17 | 1.6 | 107 |
| 218 | Discovery and Optimization of Materials Using Evolutionary Approaches. *Chemical Reviews*, **2016**, 116, 6107-32 | 68.1 | 107 |
| 217 | The role of quantitative structure--activity relationships (QSAR) in biomolecular discovery. *Briefings in Bioinformatics*, **2002**, 3, 73-86 | 13.4 | 100 |
| 216 | Understanding the Roles of the "Two QSARs". *Journal of Chemical Information and Modeling*, **2016**, 56, 269-74 | 6.1 | 95 |
| 215 | Towards chromate-free corrosion inhibitors: structure–property models for organic alternatives. *Green Chemistry*, **2014**, 16, 3349-3357 | 10 | 93 |

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| 214 | 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 |
| 213 | Unzipping the role of chirality in nanoscale self-assembly of tripeptide hydrogels. *Nanoscale*, **2012**, 4, 6752-60 | 7.7 | 89 |
| 212 | Computational Modeling and Simulation of CO Capture by Aqueous Amines. *Chemical Reviews*, **2017**, 117, 9524-9593 | 68.1 | 86 |
| 211 | Ultrafast Fabrication of Covalently Cross-linked Multifunctional Graphene Oxide Monoliths. *Advanced Functional Materials*, **2014**, 24, 4915-4921 | 15.6 | 86 |
| 210 | 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 |
| 209 | Validating Eaton's Hypothesis: Cubane as a Benzene Bioisostere. *Angewandte Chemie - International Edition*, **2016**, 55, 3580-5 | 16.4 | 78 |
| 208 | Modelling and predicting the biological effects of nanomaterials. *SAR and QSAR in Environmental Research*, **2014**, 25, 161-72 | 3.5 | 74 |
| 207 | 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 |
| 206 | Classification of emergence and its relation to self-organization. *Complexity*, **2008**, 13, 10-15 | 1.6 | 68 |
| 205 | Neural networks as robust tools in drug lead discovery and development. *Molecular Biotechnology*, **2004**, 27, 139-68 | 3 | 67 |
| 204 | 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 |
| 203 | Discovery of a Novel Polymer for Human Pluripotent Stem Cell Expansion and Multilineage Differentiation. *Advanced Materials*, **2015**, 27, 4006-12 | 24 | 64 |
| 202 | Optimal Sparse Descriptor Selection for QSAR Using Bayesian Methods. *QSAR and Combinatorial Science*, **2009**, 28, 645-653 | | 56 |
| 201 | Modelling blood-brain barrier partitioning using Bayesian neural nets. *Journal of Molecular Graphics and Modelling*, **2004**, 22, 499-505 | 2.8 | 56 |
| 200 | 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 |
| 199 | New QSAR Methods Applied to Structure□Activity Mapping and Combinatorial Chemistry. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 236-242 | | 55 |
| 198 | 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 |
| 197 | Tripeptide motifs in biology: targets for peptidomimetic design. *Journal of Medicinal Chemistry*, **2011**, 54, 1111-25 | 8.3 | 51 |

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| 196 | Robust QSAR Models from Novel Descriptors and Bayesian Regularised Neural Networks. *Molecular Simulation*, **2000**, 24, 243-258 | 2 | 50 |
| 195 | Immune Modulation by Design: Using Topography to Control Human Monocyte Attachment and Macrophage Differentiation. *Advanced Science*, **2020**, 7, 1903392 | 13.6 | 48 |
| 194 | An Optimal Self-Pruning Neural Network and Nonlinear Descriptor Selection in QSAR. *QSAR and Combinatorial Science*, **2009**, 28, 1092-1097 | | 48 |
| 193 | An Experimental and Computational Approach to the Development of ZnO Nanoparticles that are Safe by Design. *Small*, **2016**, 12, 3568-77 | 11 | 47 |
| 192 | Evolving embodied intelligence from materials to machines. *Nature Machine Intelligence*, **2019**, 1, 12-19 | 22.5 | 47 |
| 191 | Aqueous solubility prediction: do crystal lattice interactions help?. *Molecular Pharmaceutics*, **2013**, 10, 2757-66 | 5.6 | 46 |
| 190 | Conformational analysis of the ergot alkaloids ergotamine and ergotaminine. *Journal of Medicinal Chemistry*, **1982**, 25, 937-42 | 8.3 | 46 |
| 189 | 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 |
| 188 | Performance of Deep and Shallow Neural Networks, the Universal Approximation Theorem, Activity Cliffs, and QSAR. *Molecular Informatics*, **2017**, 36, 1600118 | 3.8 | 44 |
| 187 | A Carbon-13 NMR Study of Carbon Dioxide Absorption and Desorption with Aqueous Amine Solutions. *Energy Procedia*, **2009**, 1, 955-962 | 2.3 | 44 |
| 186 | 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 |
| 185 | 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 |
| 184 | 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 |
| 183 | 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 |
| 182 | Relevance Vector Machines: Sparse Classification Methods for QSAR. *Journal of Chemical Information and Modeling*, **2015**, 55, 1529-34 | 6.1 | 39 |
| 181 | Modelling and Prediction of Bacterial Attachment to Polymers. *Advanced Functional Materials*, **2014**, 24, 2085-2093 | 15.6 | 38 |
| 180 | Toward a systematic exploration of nano-bio interactions. *Toxicology and Applied Pharmacology*, **2017**, 323, 66-73 | 4.6 | 37 |
| 179 | Immune-Instructive Polymers Control Macrophage Phenotype and Modulate the Foreign Body Response In Vivo. *Matter*, **2020**, 2, 1564-1581 | 12.7 | 37 |

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| 178 | Modelling human embryoid body cell adhesion to a combinatorial library of polymer surfaces. *Journal of Materials Chemistry*, **2012**, 22, 20902-20906 | | 37 |
| 177 | 5-epi-Deoxyrhamnojirimycin is a potent inhibitor of an □-rhamnosidase: 5-epi-deoxymannojirimycin is not a potent inhibitor of an □-mannosidase. *Tetrahedron: Asymmetry*, **1998**, 9, 2947-2960 | | 37 |
| 176 | A critical overview of computational approaches employed for COVID-19 drug discovery. *Chemical Society Reviews*, **2021**, 50, 9121-9151 | 58.5 | 36 |
| 175 | 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 |
| 174 | The microwave spectrum of HCN dimer. *Journal of Molecular Spectroscopy*, **1981**, 89, 352-355 | 1.3 | 35 |
| 173 | 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 |
| 172 | Role of Artificial Intelligence and Machine Learning in Nanosafety. *Small*, **2020**, 16, e2001883 | 11 | 33 |
| 171 | The diverse biological properties of the chemically inert noble gases. *Pharmacology & Therapeutics*, **2016**, 160, 44-64 | 13.9 | 31 |
| 170 | Binding inhibitors of the bacterial sliding clamp by design. *Journal of Medicinal Chemistry*, **2011**, 54, 483188 | 8 | 31 |
| 169 | Molecular modeling studies of "flap up" mannosyl cation mimics. *Journal of Medicinal Chemistry*, **1996**, 39, 4332-4 | 8.3 | 31 |
| 168 | Conducting Polymers from Polybutadiene: Molecular Configuration Effects on the Iodine-Induced Conjugation Reactions. *Macromolecules*, **1994**, 27, 6728-6735 | 5.5 | 31 |
| 167 | Towards computational design of zeolite catalysts for CO2 reduction. *RSC Advances*, **2015**, 5, 44361-44370 | 3.7 | 30 |
| 166 | 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 |
| 165 | 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 |
| 164 | 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 |
| 163 | Prediction of Broad-Spectrum Pathogen Attachment to Coating Materials for Biomedical Devices. *ACS Applied Materials & Interfaces*, **2018**, 10, 139-149 | 9.5 | 30 |
| 162 | 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 |
| 161 | Predicting the Performance of Organic Corrosion Inhibitors. *Metals*, **2017**, 7, 553 | 2.3 | 29 |

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| 160 | Predictive Bayesian neural network models of MHC class II peptide binding. *Journal of Molecular Graphics and Modelling*, **2005**, 23, 481-9 | 2.8 | 29 |
| 159 | Contrasting Effects of Nanoparticle Binding on Protein Denaturation. *Journal of Physical Chemistry C*, **2014**, 118, 22069-22078 | 3.8 | 28 |
| 158 | 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 |
| 157 | Validating Eaton's Hypothesis: Cubane as a Benzene Bioisostere. *Angewandte Chemie*, **2016**, 128, 3644-3649 | 3.8 | 28 |
| 156 | Thermostability and reversibility of silver nanoparticle-protein binding. *Physical Chemistry Chemical Physics*, **2015**, 17, 1728-39 | 3.6 | 26 |
| 155 | Accurate and interpretable nanoSAR models from genetic programming-based decision tree construction approaches. *Nanotoxicology*, **2016**, 10, 1001-12 | 5.3 | 26 |
| 154 | Probing enzyme-nanoparticle interactions using combinatorial gold nanoparticle libraries. *Nano Research*, **2015**, 8, 1293-1308 | 10 | 26 |
| 153 | Toward novel universal descriptors: charge fingerprints. *Journal of Chemical Information and Modeling*, **2009**, 49, 710-5 | 6.1 | 26 |
| 152 | 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 |
| 151 | Critical-like self-organization and natural selection: two facets of a single evolutionary process?. *BioSystems*, **2008**, 92, 148-58 | 1.9 | 26 |
| 150 | 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 |
| 149 | Robust modelling of solubility in supercritical carbon dioxide using Bayesian methods. *Journal of Molecular Graphics and Modelling*, **2010**, 28, 593-7 | 2.8 | 25 |
| 148 | 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 |
| 147 | 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 |
| 146 | Targeted cytotoxic cells as a novel form of cancer immunotherapy. *Molecular Immunology*, **1988**, 25, 1099-103 | 4.3 | 25 |
| 145 | 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 |
| 144 | Neural networks in ADME and toxicity prediction. *Drugs of the Future*, **2004**, 29, 1043 | 2.3 | 23 |
| 143 | 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 |

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| 142 | Bayesian neural nets for modeling in drug discovery. *Drug Discovery Today Biosilico*, **2004**, 2, 104-111 | | 21 |
| 141 | Quantitative design rules for protein-resistant surface coatings using machine learning. *Scientific Reports*, **2019**, 9, 265 | 4.9 | 20 |
| 140 | Machine learning property prediction for organic photovoltaic devices. *Npj Computational Materials* , **2020**, 6, | 10.9 | 20 |
| 139 | Atomistic Topological Indices Applied to Benzodiazepines using Various Regression Methods. *QSAR and Combinatorial Science*, **1998**, 17, 14-19 | | 20 |
| 138 | Predictive Human Intestinal Absorption QSAR Models Using Bayesian Regularized Neural Networks. *Australian Journal of Chemistry*, **2005**, 58, 859 | 1.2 | 20 |
| 137 | In silico screening of modulators of magnesium dissolution. *Corrosion Science*, **2020**, 163, 108245 | 6.8 | 20 |
| 136 | Holographic QSAR of Benzodiazepines. *QSAR and Combinatorial Science*, **1998**, 17, 224-231 | | 20 |
| 135 | A thrombopoietin receptor antagonist is capable of depleting myelofibrosis hematopoietic stem and progenitor cells. *Blood*, **2016**, 127, 3398-409 | 2.2 | 19 |
| 134 | Piperidine analogues of D-galactose as potent inhibitors of β-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 |
| 133 | π-Doping of 1,4-polydienes. *Synthetic Metals*, **1995**, 69, 563-566 | 3.6 | 19 |
| 132 | Predicting the complex phase behavior of self-assembling drug delivery nanoparticles. *Molecular Pharmaceutics*, **2013**, 10, 1368-77 | 5.6 | 18 |
| 131 | Optimal machine learning models for robust materials classification using ToF-SIMS data. *Applied Surface Science*, **2019**, 487, 773-783 | 6.7 | 17 |
| 130 | Discovery of (meth)acrylate polymers that resist colonization by fungi associated with pathogenesis and biodeterioration. *Science Advances*, **2020**, 6, eaba6574 | 14.3 | 17 |
| 129 | Multivariate analysis of ToF-SIMS data using mass segmented peak lists. *Surface and Interface Analysis*, **2018**, 50, 713-728 | 1.5 | 17 |
| 128 | Definitive confirmation for through-space bond dominance in the outermost π orbitals of norbornadiene. *Journal of Electron Spectroscopy and Related Phenomena*, **2002**, 123, 389-395 | 1.7 | 17 |
| 127 | Hyperfine interactions in methanimine. *Australian Journal of Chemistry*, **1982**, 35, 667 | 1.2 | 17 |
| 126 | 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 |
| 125 | Self-organizing circuitry and emergent computation in mouse embryonic stem cells. *Stem Cell Research*, **2012**, 8, 324-33 | 1.6 | 16 |

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| 124 | Stem cell decision making and critical-like exploratory networks. *Stem Cell Research*, **2009**, 2, 165-77 | 1.6 | 16 |
| 123 | Predicting maximum bioactivity by effective inversion of neural networks using genetic algorithms. *Chemometrics and Intelligent Laboratory Systems*, **1997**, 38, 127-137 | 3.8 | 16 |
| 122 | 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 |
| 121 | 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 |
| 120 | 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 |
| 119 | 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 |
| 118 | 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 |
| 117 | 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 |
| 116 | A Bright Future for Evolutionary Methods in Drug Design. *ChemMedChem*, **2015**, 10, 1296-300 | 3.7 | 15 |
| 115 | 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 |
| 114 | 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 |
| 113 | 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 |
| 112 | Antifibrotic strategies for medical devices. *Advanced Drug Delivery Reviews*, **2020**, 167, 109-120 | 18.5 | 14 |
| 111 | Potential intermediates for incorporation of polyhydroxylated prolines into combinatorial libraries. *Tetrahedron Letters*, **1998**, 39, 6091-6094 | 2 | 14 |
| 110 | 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 |
| 109 | A conformational study of the topographical requirements of a phytotropin recognition site on the naphthylphthalamic acid receptor. *Phytochemistry*, **1987**, 26, 2881-2889 | 4 | 14 |
| 108 | Predicting Thermal Properties of Crystals Using Machine Learning. *Advanced Theory and Simulations* , **2020**, 3, 1900208 | 3.5 | 14 |
| 107 | Toward Interpretable Machine Learning Models for Materials Discovery. *Advanced Intelligent Systems*, **2019**, 1, 1900045 | 6 | 14 |

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| 106 | 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 |
| 105 | Structure and Function of Ecdysone Receptors I. Interactions with Ecdysteroids and Synthetic Agonists. *Advances in Insect Physiology*, **2012**, 43, 299-351 | 2.5 | 13 |
| 104 | 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 |
| 103 | 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 |
| 102 | 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 |
| 101 | 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 |
| 100 | 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 |
| 99 | Sparse QSAR modelling methods for therapeutic and regenerative medicine. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 497-509 | 4.2 | 11 |
| 98 | Hyperfine interactions in the microwave spectrum of 2-propen-1-Imine (vinylimine). *Chemical Physics*, **1981**, 59, 243-247 | 2.3 | 11 |
| 97 | 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 |
| 96 | 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 |
| 95 | Application of neural networks to large dataset QSAR, virtual screening, and library design. *Methods in Molecular Biology*, **2002**, 201, 325-67 | 1.4 | 10 |
| 94 | 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 |
| 93 | The microwave spectrum of (Z)-Ethanimine. *Australian Journal of Chemistry*, **1980**, 33, 1 | 1.2 | 10 |
| 92 | 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 |
| 91 | Application of DFT and EMS to the Study of Strained Organic Molecules. *Australian Journal of Physics*, **1998**, 51, 707 | | 9 |
| 90 | 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 |
| 89 | Hydration and Dynamics of Ligands Determine the Antifouling Capacity of Functionalized Surfaces. *Journal of Physical Chemistry C*, **2019**, 123, 30360-30372 | 3.8 | 9 |

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| 88 | Immobilisation of a thrombopoietin peptidic mimic by self-assembled monolayers for culture of CD34+ cells. *Biomaterials*, **2015**, 37, 82-93 | 15.6 | 8 |
| 87 | Modeling the Influence of Fatty Acid Incorporation on Mesophase Formation in Amphiphilic Therapeutic Delivery Systems. *Molecular Pharmaceutics*, **2016**, 13, 996-1003 | 5.6 | 8 |
| 86 | Getting to the source: selective drug targeting of cancer stem cells. *ChemMedChem*, **2014**, 9, 885-98 | 3.7 | 8 |
| 85 | Robust, quantitative tools for modelling ex-vivo expansion of haematopoietic stem cells and progenitors. *Molecular BioSystems*, **2012**, 8, 913-20 | | 8 |
| 84 | Principal signalling complexes in haematopoiesis: structural aspects and mimetic discovery. *Cytokine and Growth Factor Reviews*, **2011**, 22, 231-53 | 17.9 | 8 |
| 83 | 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 |
| 82 | Synthesis, Biological Activity, and QSAR Studies of Antimicrobial Agents Containing Biguanide Isosteres. *Australian Journal of Chemistry*, **2004**, 57, 77 | 1.2 | 8 |
| 81 | 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 |
| 80 | Morpheus: a conformation-activity relationships and receptor modeling package. *Journal of Molecular Graphics*, **1989**, 7, 138-45 | | 8 |
| 79 | 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 |
| 78 | Computational Modelling of Magnetic Nanoparticle Properties and In Vivo Responses. *Current Medicinal Chemistry*, **2017**, 24, 483-496 | 4.3 | 8 |
| 77 | Ligand Entropy Is Hard but Should Not Be Ignored. *Journal of Chemical Information and Modeling*, **2020**, 60, 4421-4423 | 6.1 | 8 |
| 76 | Use of Artificial Intelligence and Machine Learning for Discovery of Drugs for Neglected Tropical Diseases. *Frontiers in Chemistry*, **2021**, 9, 614073 | 5 | 8 |
| 75 | Glossary of terms used in computational drug design, part II (IUPAC Recommendations 2015). *Pure and Applied Chemistry*, **2016**, 88, 239-264 | 2.1 | 8 |
| 74 | Modelling atypical small-molecule mimics of an important stem cell cytokine, thrombopoietin. *ChemMedChem*, **2009**, 4, 2002-11 | 3.7 | 7 |
| 73 | Transformation of substituted 2H-pyran-5-carboxylates into 3R*-vinyl-1,2R*-cyclopropanedicarboxylates. *New Journal of Chemistry*, **1998**, 22, 1485-1492 | 3.6 | 7 |
| 72 | The non-Fickian diffusion of deterrents into a nitrocellulose-based propellant. *Journal of Applied Polymer Science*, **1988**, 35, 51-62 | 2.9 | 7 |
| 71 | Coatings Releasing the Relaxin Peptide Analogue B7-33 Reduce Fibrotic Encapsulation. *ACS Applied Materials & Interfaces*, **2019**, 11, 45511-45519 | 9.5 | 6 |

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| 70 | Modeling the molecular basis for α4β1 integrin antagonism. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 5903-11 | 3.4 | 6 |
| 69 | Modelling topoisomerase I inhibition by minor groove binders. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 1450-7 | 3.4 | 6 |
| 68 | Modelling inhalational anaesthetics using bayesian feature selection and QSAR modelling methods. *ChemMedChem*, **2010**, 5, 1318-23 | 3.7 | 6 |
| 67 | Parasiticidal 2-alkoxy- and 2-aryloxyiminoalkyl trifluoromethanesulfonanilides. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 252-5 | 2.9 | 6 |
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