

Robert J Doerksen

List of Publications by Year in Descending Order

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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.

103
papers

4,922
citations

26
h-index

69
g-index

104
ext. papers

5,365
ext. citations

4.7
avg, IF

5.04
L-index

#	Paper	IF	Citations
103	Fractionation of sulfated galactan from the red alga <i>Botryocladia occidentalis</i> separates its anticoagulant and anti-SARS-CoV-2 properties.. <i>Journal of Biological Chemistry</i> , 2022 , 101856	5.4	1
102	Validated determination of NRG1 Ig-like domain structure by mass spectrometry coupled with computational modeling.. <i>Communications Biology</i> , 2022 , 5, 452	6.7	1
101	Optimization of sulfobutyl-ether- β -cyclodextrin levels in oral formulations to enhance progesterone bioavailability. <i>International Journal of Pharmaceutics</i> , 2021 , 596, 120212	6.5	6
100	Enantioselective Interactions of Anti-Infective 8-Aminoquinoline Therapeutics with Human Monoamine Oxidases A and B. <i>Pharmaceutics</i> , 2021 , 14,	5.2	2
99	Negative allosteric modulators of cannabinoid receptor 1: Ternary complexes including CB1, orthosteric CP55940 and allosteric ORG27569. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-19	3.6	2
98	Structural and kinetic analyses of holothurian sulfated glycans suggest potential treatment for SARS-CoV-2 infection. <i>Journal of Biological Chemistry</i> , 2021 , 297, 101207	5.4	7
97	Identification of potential non-nucleoside MraY inhibitors for tuberculosis chemotherapy using structure-based virtual screening. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-18	3.6	16
96	Hypervalent Iodine Mediated Oxidative Cyclization of Acrylamide -Carbamates to 5,5-Disubstituted Oxazolidine-2,4-diones. <i>Journal of Organic Chemistry</i> , 2020 , 85, 7549-7557	4.2	4
95	Identification of a novel umami peptide in tempeh (Indonesian fermented soybean) and its binding mechanism to the umami receptor T1R. <i>Food Chemistry</i> , 2020 , 333, 127411	8.5	10
94	Design, synthesis and biological evaluation of novel naturally-inspired multifunctional molecules for the management of Alzheimer's disease. <i>European Journal of Medicinal Chemistry</i> , 2020 , 198, 112257	6.8	15
93	Puupehenone, a Marine-Sponge-Derived Sesquiterpene Quinone, Potentiates the Antifungal Drug Caspofungin by Disrupting Hsp90 Activity and the Cell Wall Integrity Pathway. <i>MSphere</i> , 2020 , 5,	5	8
92	Conformational properties of l-fucose and the tetrasaccharide building block of the sulfated l-fucan from <i>Lytechinus variegatus</i> . <i>Journal of Structural Biology</i> , 2020 , 209, 107407	3.4	4
91	Potential Modulation of Human NAD[P]H-Quinone Oxidoreductase 1 (NQO1) by EGCG and Its Metabolites-A Systematic Computational Study. <i>Chemical Research in Toxicology</i> , 2020 , 33, 2749-2764	4	2
90	Selective Interactions of -Methylated Flavonoid Natural Products with Human Monoamine Oxidase-A and -B. <i>Molecules</i> , 2020 , 25,	4.8	5
89	Negative allosteric modulators of cannabinoid receptor 2: protein modeling, binding site identification and molecular dynamics simulations in the presence of an orthosteric agonist. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 32-47	3.6	16
88	Hepatoprotective Tetrahydrobenzocyclooctabenzofuranone Lignans from. <i>Journal of Natural Products</i> , 2019 , 82, 2842-2851	4.9	5
87	Salvindolin elicits opioid system-mediated antinociceptive and antidepressant-like activities. <i>Journal of Psychopharmacology</i> , 2019 , 33, 865-881	4.6	6

86	Selective Inhibition of Human Monoamine Oxidase B by Acacetin 7-Methyl Ether Isolated from (Damiana). <i>Molecules</i> , 2019 , 24,	4.8	21
85	Computationally Assisted Discovery and Assignment of a Highly Strained and PANC-1 Selective Alkaloid from Alaska's Deep Ocean. <i>Journal of the American Chemical Society</i> , 2019 , 141, 4338-4344	16.4	28
84	Agonists of the γ -Aminobutyric acid type B (GABA) receptor derived from β -hydroxy and β -amino difluoromethyl ketones. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2018 , 28, 2697-2700	2.9	6
83	Antimalarial naphthoquinones. Synthesis via click chemistry, in vitro activity, docking to PfDHODH and SAR of lapachol-based compounds. <i>European Journal of Medicinal Chemistry</i> , 2018 , 145, 191-205	6.8	45
82	Hepatoprotective Dibenzocyclooctadiene and Tetrahydrobenzocyclooctabenzofuranone Lignans from <i>Kadsura longipedunculata</i> . <i>Journal of Natural Products</i> , 2018 , 81, 846-857	4.9	15
81	Selective Cannabinoid 2 Receptor Stimulation Reduces Tubular Epithelial Cell Damage after Renal Ischemia-Reperfusion Injury. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2018 , 364, 287-299	4.7	18
80	Antileishmanial Carbasugars from <i>Geosmithia langdonii</i> . <i>Journal of Natural Products</i> , 2018 , 81, 2222-2227	4.9	5
79	Structure-Based Identification of Potent Natural Product Chemotypes as Cannabinoid Receptor 1 Inverse Agonists. <i>Molecules</i> , 2018 , 23,	4.8	8
78	Computationally Assisted Assignment of the <i>Kadsuraols</i> , a Class of Chemopreventive Agents for the Control of Liver Cancer. <i>Organic Letters</i> , 2018 , 20, 5559-5563	6.2	15
77	Interactions of endocannabinoid virodhamine and related analogs with human monoamine oxidase-A and -B. <i>Biochemical Pharmacology</i> , 2018 , 155, 82-91	6	9
76	Assignment of the absolute configuration of hepatoprotective highly oxygenated triterpenoids using X-ray, ECD, NMR J-based configurational analysis and HSQC overlay experiments. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017 , 1861, 3089-3095	4	12
75	In silico investigation of lavandulyl flavonoids for the development of potent fatty acid synthase-inhibitory prototypes. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2017 , 1861, 3180-3188	4	10
74	Clotrimazole-cyclodextrin based approach for the management and treatment of Candidiasis - A formulation and chemistry-based evaluation. <i>Pharmaceutical Development and Technology</i> , 2016 , 21, 619-29	3.4	19
73	Methemoglobinemia Hemotoxicity of Some Antimalarial 8-Aminoquinoline Analogues and Their Hydroxylated Derivatives: Density Functional Theory Computation of Ionization Potentials. <i>Chemical Research in Toxicology</i> , 2016 , 29, 1132-41	4	2
72	New Drugs from Natural Products around the World 2016 , 22, 215-216		4
71	Screening and profiling stilbene-type natural products with angiotensin-converting enzyme inhibitory activity from <i>Ampelopsis brevipedunculata</i> var. <i>hancei</i> (Planch.) Rehder. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2015 , 108, 70-7	3.5	14
70	Nitroreductase-triggered activation of a novel caged fluorescent probe obtained from methylene blue. <i>Chemical Communications</i> , 2015 , 51, 12787-90	5.8	76
69	Activation of the γ -Aminobutyric Acid Type B (GABA(B)) Receptor by Agonists and Positive Allosteric Modulators. <i>Journal of Medicinal Chemistry</i> , 2015 , 58, 6336-47	8.3	25

68	Screening, discovery, and characterization of angiotensin-I converting enzyme inhibitory peptides derived from proteolytic hydrolysate of bitter melon seed proteins. <i>Journal of Proteomics</i> , 2015 , 128, 424-35	3.9	50
67	Data in support of optimized production of angiotensin-I converting enzyme inhibitory peptides derived from proteolytic hydrolysate of bitter melon seed proteins. <i>Data in Brief</i> , 2015 , 5, 403-7	1.2	1
66	Andrographolide induces apoptosis via down-regulation of glyoxalase 1 and HMG-CoA reductase in HL-60 cells. <i>Journal of Functional Foods</i> , 2015 , 14, 226-235	5.1	8
65	Computational Study on the Effect of Exocyclic Substituents on the Ionization Potential of Primaquine: Insights into the Design of Primaquine-Based Antimalarial Drugs with Less Methemoglobin Generation. <i>Chemical Research in Toxicology</i> , 2015 , 28, 169-74	4	6
64	Quinone propionic acid-based redox-triggered polymer nanoparticles for drug delivery: Computational analysis and in vitro evaluation. <i>Journal of Applied Polymer Science</i> , 2014 , 131, n/a-n/a	2.9	6
63	Discovery of thienoquinolone derivatives as selective and ATP non-competitive CDK5/p25 inhibitors by structure-based virtual screening. <i>Bioorganic and Medicinal Chemistry</i> , 2014 , 22, 6409-21	3.4	25
62	Hydroxylated derivatives of NPC1161: theoretical insights into their potential toxicity and the feasibility and regioselectivity of their formation. <i>Journal of Physical Chemistry A</i> , 2014 , 118, 5501-7	2.8	3
61	Asphodosides A-E, anti-MRSA metabolites from <i>Asphodelus microcarpus</i> . <i>Phytochemistry</i> , 2014 , 105, 79-84	4	6
60	Isolation and characterization of new secondary metabolites from. <i>Medicinal Chemistry Research</i> , 2014 , 23, 3510-3515	2.2	6
59	Structure of the cannabinoid receptor 1: homology modeling of its inactive state and enrichment study based on CB1 antagonist docking. <i>MedChemComm</i> , 2014 , 5, 1297-1302	5	6
58	Pharmacophore Modeling, Ensemble Docking, Virtual Screening, and Biological Evaluation on Glycogen Synthase Kinase-3. <i>Molecular Informatics</i> , 2014 , 33, 610-26	3.8	11
57	Quantitative Structure-Activity Relationship Analysis and a Combined Ligand-Based/Structure-Based Virtual Screening Study for Glycogen Synthase Kinase-3. <i>Molecular Informatics</i> , 2014 , 33, 627-40	3.8	7
56	Drug activity prediction using multiple-instance learning via joint instance and feature selection. <i>BMC Bioinformatics</i> , 2013 , 14 Suppl 14, S16	3.6	15
55	Computationally assisted assignment of kahalalide Y configuration using an NMR-constrained conformational search. <i>Journal of Natural Products</i> , 2013 , 76, 178-85	4.9	8
54	A novel natural phenyl alkene with cytotoxic activity. <i>Tetrahedron Letters</i> , 2013 , 54, 3872-3876	2	12
53	Configurational assignments of conformationally restricted bis-monoterpene hydroquinones: utility in exploration of endangered plants. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2013 , 1830, 4229-34	4	5
52	Docking challenge: protein sampling and molecular docking performance. <i>Journal of Chemical Information and Modeling</i> , 2013 , 53, 1934-45	6.1	127
51	Effect of antimalarial drug primaquine and its derivatives on the ionization potential of hemoglobin: A QM/MM study. <i>MedChemComm</i> , 2013 , 4, 1145-1147	5	6

50	Methemoglobin generation by 8-aminoquinolines: effect of substitution at 5-position of primaquine. <i>Chemical Research in Toxicology</i> , 2013 , 26, 1801-9	4	6
49	Significance of endangered and threatened plant natural products in the control of human disease. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013 , 110, 16832-7	11.5	53
48	Quantitative structure-activity relationships of imidazole-containing farnesyltransferase inhibitors using different chemometric methods. <i>Medicinal Chemistry</i> , 2013 , 9, 434-48	1.8	9
47	Combined rule extraction and feature elimination in supervised classification. <i>IEEE Transactions on Nanobioscience</i> , 2012 , 11, 228-36	3.4	18
46	Natural prenylated resveratrol analogs arachidin-1 and -3 demonstrate improved glucuronidation profiles and have affinity for cannabinoid receptors. <i>Xenobiotica</i> , 2012 , 42, 139-56	2	34
45	Molecular modeling to provide insight into the substrate binding and catalytic mechanism of human biliverdin-IXβ reductase. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 9580-94	3.4	25
44	Implementation of multiple-instance learning in drug activity prediction. <i>BMC Bioinformatics</i> , 2012 , 13 Suppl 15, S3	3.6	13
43	Methemoglobinemia caused by 8-aminoquinoline drugs: DFT calculations suggest an analogy to H4BB role in nitric oxide synthase. <i>Journal of the American Chemical Society</i> , 2011 , 133, 1172-5	16.4	16
42	Computational Study on the Conformations of Gambogic Acid. <i>Chemical Physics Letters</i> , 2011 , 511, 405-413	4.3	1
41	Leveraging domain information to restructure biological prediction. <i>BMC Bioinformatics</i> , 2011 , 12 Suppl 10, S22	3.6	0
40	Multi-class Joint Rule Extraction and Feature Selection for Biological Data 2011 ,		4
39	DFT study on the radical anions formed by primaquine and its derivatives. <i>Chemical Research in Toxicology</i> , 2011 , 24, 1476-85	4	11
38	Assignment of absolute configuration of sulfinyl dilactones: Optical rotations and 1H NMR experiment and DFT calculations. <i>Journal of Molecular Structure</i> , 2011 , 987, 166-173	3.4	7
37	Template-based protein modeling: recent methodological advances. <i>Current Topics in Medicinal Chemistry</i> , 2010 , 10, 84-94	3	33
36	Protein kinase-inhibitor database: structural variability of and inhibitor interactions with the protein kinase P-loop. <i>Journal of Proteome Research</i> , 2010 , 9, 4433-42	5.6	38
35	Structure-activity relationship and mechanism of action studies of manzamine analogues for the control of neuroinflammation and cerebral infections. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 61-76	8.3	70
34	Polyketide-peroxides from a Species of Jamaican Plakortis (Porifera: Demospongiae). <i>Australian Journal of Chemistry</i> , 2010 , 63, 877	1.2	20
33	Computational Study on the Conformations of Mitragynine and Mitragynaline. <i>Computational and Theoretical Chemistry</i> , 2010 , 945, 57-63		7

32	Biochemical and structural consequences of a glycine deletion in the alpha-8 helix of protoporphyrinogen oxidase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2010 , 1804, 1548-56	4	44
31	Computational model of hepatitis B virus DNA polymerase: molecular dynamics and docking to understand resistant mutations. <i>Protein Science</i> , 2010 , 19, 796-807	6.3	34
30	Three-dimensional quantitative structure-farnesyltransferase inhibition analysis for some diaminobenzophenones. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2009 , 24, 1220-8	5.6	3
29	Topological polar surface area: a useful descriptor in 2D-QSAR. <i>Current Medicinal Chemistry</i> , 2009 , 16, 21-41	4.3	107
28	Semisynthetic latrunculin B analogs: studies of actin docking support a proposed mechanism for latrunculin bioactivity. <i>Bioorganic and Medicinal Chemistry</i> , 2009 , 17, 7517-22	3.4	9
27	Glycogen synthase kinase-3 inhibition by 3-anilino-4-phenylmaleimides: insights from 3D-QSAR and docking. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 113-27	4.2	17
26	Imidazole-containing farnesyltransferase inhibitors: 3D quantitative structure-activity relationships and molecular docking. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 431-48	4.2	12
25	Structure-activity relationship and comparative docking studies for cycloguanil analogs as PFDHFR-TS inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1787-96	6.1	20
24	Stereoelectronic properties of spiroquinazolinones in differential PDE7 inhibitory activity. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1945-54	3.5	25
23	2-N-Methyl modifications and SAR studies of manzamine A. <i>Bioorganic and Medicinal Chemistry</i> , 2008 , 16, 6702-6	3.4	24
22	Latrunculin with a highly oxidized thiazolidinone ring: structure assignment and actin docking. <i>Organic Letters</i> , 2007 , 9, 4773-6	6.2	26
21	3D-QSAR analysis of antimalarial farnesyltransferase inhibitors based on a 2,5-diaminobenzophenone scaffold. <i>Bioorganic and Medicinal Chemistry</i> , 2006 , 14, 7311-23	3.4	19
20	Probing the physicochemical and structural requirements for glycogen synthase kinase-3alpha inhibition: 2D-QSAR for 3-anilino-4-phenylmaleimides. <i>Bioorganic and Medicinal Chemistry</i> , 2006 , 14, 8210-8	3.4	28
19	Biomimetic facially amphiphilic antibacterial oligomers with conformationally stiff backbones. <i>Chemistry and Biology</i> , 2006 , 13, 427-35		70
18	Advances in methods and algorithms in a modern quantum chemistry program package. <i>Physical Chemistry Chemical Physics</i> , 2006 , 8, 3172-91	3.6	2371
17	Synthesis of urea oligomers and their antibacterial activity. <i>Chemical Communications</i> , 2005 , 1537-9	5.8	64
16	Are polarizabilities useful as aromaticity indices? Tests on azines, azoles, oxazoles and thiazoles. <i>Journal of Computational Methods in Sciences and Engineering</i> , 2004 , 4, 427-438	0.3	3
15	Nontoxic membrane-active antimicrobial arylamide oligomers. <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 1158-62	16.4	189

14	Cover Picture: Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers (Angew. Chem. Int. Ed. 9/2004). <i>Angewandte Chemie - International Edition</i> , 2004 , 43, 1033-1033	16.4	1
13	Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers. <i>Angewandte Chemie</i> , 2004 , 116, 1178-1182	3.6	29
12	Titelbild: Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers (Angew. Chem. 9/2004). <i>Angewandte Chemie</i> , 2004 , 116, 1051-1051	3.6	
11	Controlling the conformation of arylamides: computational studies of intramolecular hydrogen bonds between amides and ethers or thioethers. <i>Chemistry - A European Journal</i> , 2004 , 10, 5008-16	4.8	35
10	Intramolecular hydrogen bonds: ab initio CarParrinello simulations of arylamide torsions. <i>Chemical Physics Letters</i> , 2003 , 380, 150-157	2.5	13
9	Novel conformationally-constrained beta-peptides characterized by 1H NMR chemical shifts. <i>Chemical Communications</i> , 2003 , 2534-5	5.8	38
8	Bond orders in heteroaromatic rings*. <i>International Journal of Quantum Chemistry</i> , 2002 , 90, 534-540	2.1	25
7	De novo design of biomimetic antimicrobial polymers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002 , 99, 5110-4	11.5	387
6	Geometries and multipole moments of AlH ₄ SiH ₄ , PH ₃ , H ₂ S and HCl. <i>Computational and Theoretical Chemistry</i> , 1999 , 488, 217-221		10
5	Structures, Vibrational Frequencies and Polarizabilities of Diazaborinines, Triazadiborinines, Azaboroles, and Oxazaboroles. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 2141-2151	2.8	31
4	Quadrupole and Octopole Moments of Heteroaromatic Rings. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 10009-10014	2.8	62
3	Azaborinines: Structures, Vibrational Frequencies, and Polarizabilities. <i>Journal of Physical Chemistry A</i> , 1998 , 102, 4679-4686	2.8	21
2	Polarizabilities of Oxazoles: Ab Initio Calculations and Simple Models. <i>The Journal of Physical Chemistry</i> , 1996 , 100, 8752-8757		37
1	Polarizabilities of Aromatic Five-Membered Rings: Azoles. <i>The Journal of Physical Chemistry</i> , 1995 , 99, 12790-12796		53