Robert J Doerksen

List of Publications by Citations

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	Advances in methods and algorithms in a modern quantum chemistry program package. *Physical Chemistry Chemical Physics*, **2006**, 8, 3172-91	3.6	2371
102	De novo design of biomimetic antimicrobial polymers. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 5110-4	11.5	387
101	Nontoxic membrane-active antimicrobial arylamide oligomers. *Angewandte Chemie - International Edition*, **2004**, 43, 1158-62	16.4	189
100	Docking challenge: protein sampling and molecular docking performance. *Journal of Chemical Information and Modeling*, **2013**, 53, 1934-45	6.1	127
99	Topological polar surface area: a useful descriptor in 2D-QSAR. *Current Medicinal Chemistry*, **2009**, 16, 21-41	4.3	107
98	Nitroreductase-triggered activation of a novel caged fluorescent probe obtained from methylene blue. *Chemical Communications*, **2015**, 51, 12787-90	5.8	76
97	Structure-activity relationship and mechanism of action studies of manzamine analogues for the control of neuroinflammation and cerebral infections. *Journal of Medicinal Chemistry*, **2010**, 53, 61-76	8.3	70
96	Biomimetic facially amphiphilic antibacterial oligomers with conformationally stiff backbones. *Chemistry and Biology*, **2006**, 13, 427-35		70
95	Synthesis of urea oligomers and their antibacterial activity. *Chemical Communications*, **2005**, 1537-9	5.8	64
94	Quadrupole and Octopole Moments of Heteroaromatic Rings. *Journal of Physical Chemistry A*, **1999**, 103, 10009-10014	2.8	62
93	Significance of endangered and threatened plant natural products in the control of human disease. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 16832-7	11.5	53
92	Polarizabilities of Aromatic Five-Membered Rings: Azoles. *The Journal of Physical Chemistry*, **1995**, 99, 12790-12796		53
91	Screening, discovery, and characterization of angiotensin-I converting enzyme inhibitory peptides derived from proteolytic hydrolysate of bitter melon seed proteins. *Journal of Proteomics*, **2015**, 128, 424-35	3.9	50
90	Antimalarial naphthoquinones. Synthesis via click chemistry, in vitro activity, docking to PfDHODH and SAR of lapachol-based compounds. *European Journal of Medicinal Chemistry*, **2018**, 145, 191-205	6.8	45
89	Biochemical and structural consequences of a glycine deletion in the alpha-8 helix of protoporphyrinogen oxidase. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2010**, 1804, 1548-56	4	44
88	Protein kinase-inhibitor database: structural variability of and inhibitor interactions with the protein kinase P-loop. *Journal of Proteome Research*, **2010**, 9, 4433-42	5.6	38
87	Novel conformationally-constrained beta-peptides characterized by 1H NMR chemical shifts. *Chemical Communications*, **2003**, 2534-5	5.8	38

86	Polarizabilities of Oxazoles:Ab Initio Calculations and Simple Models. *The Journal of Physical Chemistry*, **1996**, 100, 8752-8757		37
85	Controlling the conformation of arylamides: computational studies of intramolecular hydrogen bonds between amides and ethers or thioethers. *Chemistry - A European Journal*, **2004**, 10, 5008-16	4.8	35
84	Natural prenylated resveratrol analogs arachidin-1 and -3 demonstrate improved glucuronidation profiles and have affinity for cannabinoid receptors. *Xenobiotica*, **2012**, 42, 139-56	2	34
83	Computational model of hepatitis B virus DNA polymerase: molecular dynamics and docking to understand resistant mutations. *Protein Science*, **2010**, 19, 796-807	6.3	34
82	Template-based protein modeling: recent methodological advances. *Current Topics in Medicinal Chemistry*, **2010**, 10, 84-94	3	33
81	Structures, Vibrational Frequencies and Polarizabilities of Diazaborinines, Triazadiborinines, Azaboroles, and Oxazaboroles. *Journal of Physical Chemistry A*, **1999**, 103, 2141-2151	2.8	31
80	Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers. *Angewandte Chemie*, **2004**, 116, 1178-1182	3.2	29
79	Probing the physicochemical and structural requirements for glycogen synthase kinase-3alpha inhibition: 2D-QSAR for 3-anilino-4-phenylmaleimides. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 8210-8	3.4	28
78	Computationally Assisted Discovery and Assignment of a Highly Strained and PANC-1 Selective Alkaloid from Alaskan Deep Ocean. *Journal of the American Chemical Society*, **2019**, 141, 4338-4344	16.4	28
77	Latrunculin with a highly oxidized thiazolidinone ring: structure assignment and actin docking. *Organic Letters*, **2007**, 9, 4773-6	6.2	26
76	Activation of the Aminobutyric Acid Type B (GABA(B)) Receptor by Agonists and Positive Allosteric Modulators. *Journal of Medicinal Chemistry*, **2015**, 58, 6336-47	8.3	25
75	Discovery of thienoquinolone derivatives as selective and ATP non-competitive CDK5/p25 inhibitors by structure-based virtual screening. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 6409-21	3.4	25
74	Molecular modeling to provide insight into the substrate binding and catalytic mechanism of human biliverdin-IX reductase. *Journal of Physical Chemistry B*, **2012**, 116, 9580-94	3.4	25
73	Stereoelectronic properties of spiroquinazolinones in differential PDE7 inhibitory activity. *Journal of Computational Chemistry*, **2008**, 29, 1945-54	3.5	25
72	Bond orders in heteroaromatic rings*. *International Journal of Quantum Chemistry*, **2002**, 90, 534-540	2.1	25
71	2-N-Methyl modifications and SAR studies of manzamine A. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 6702-6	3.4	24
70	Selective Inhibition of Human Monoamine Oxidase B by Acacetin 7-Methyl Ether Isolated from (Damiana). *Molecules*, **2019**, 24,	4.8	21
69	Azaborinines:Structures, Vibrational Frequencies, and Polarizabilities. *Journal of Physical Chemistry A*, **1998**, 102, 4679-4686	2.8	21

68	Polyketide-peroxides from a Species of Jamaican Plakortis (Porifera: Demospongiae). *Australian Journal of Chemistry*, **2010**, 63, 877	1.2	20
67	Structure-activity relationship and comparative docking studies for cycloguanil analogs as PfDHFR-TS inhibitors. *Journal of Chemical Information and Modeling*, **2009**, 49, 1787-96	6.1	20
66	Clotrimazole-cyclodextrin based approach for the management and treatment of Candidiasis - A formulation and chemistry-based evaluation. *Pharmaceutical Development and Technology*, **2016**, 21, 619-29	3.4	19
65	3D-QSAR analysis of antimalarial farnesyltransferase inhibitors based on a 2,5-diaminobenzophenone scaffold. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 7311-23	3.4	19
64	Combined rule extraction and feature elimination in supervised classification. *IEEE Transactions on Nanobioscience*, **2012**, 11, 228-36	3.4	18
63	Selective Cannabinoid 2 Receptor Stimulation Reduces Tubular Epithelial Cell Damage after Renal Ischemia-Reperfusion Injury. *Journal of Pharmacology and Experimental Therapeutics*, **2018**, 364, 287-299	4.7	18
62	Glycogen synthase kinase-3 inhibition by 3-anilino-4-phenylmaleimides: insights from 3D-QSAR and docking. *Journal of Computer-Aided Molecular Design*, **2009**, 23, 113-27	4.2	17
61	Identification of potential non-nucleoside MraY inhibitors for tuberculosis chemotherapy using structure-based virtual screening. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-18	3.6	16
60	Methemoglobinemia caused by 8-aminoquinoline drugs: DFT calculations suggest an analogy to H4BR's role in nitric oxide synthase. *Journal of the American Chemical Society*, **2011**, 133, 1172-5	16.4	16
59	Negative allosteric modulators of cannabinoid receptor 2: protein modeling, binding site identification and molecular dynamics simulations in the presence of an orthosteric agonist. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 32-47	3.6	16
58	Design, synthesis and biological evaluation of novel naturally-inspired multifunctional molecules for the management of Alzheimer's disease. *European Journal of Medicinal Chemistry*, **2020**, 198, 112257	6.8	15
57	Hepatoprotective Dibenzocyclooctadiene and Tetrahydrobenzocyclooctabenzofuranone Lignans from Kadsura longipedunculata. *Journal of Natural Products*, **2018**, 81, 846-857	4.9	15
56	Drug activity prediction using multiple-instance learning via joint instance and feature selection. *BMC Bioinformatics*, **2013**, 14 Suppl 14, S16	3.6	15
55	Computationally Assisted Assignment of the Kadsuraols, a Class of Chemopreventive Agents for the Control of Liver Cancer. *Organic Letters*, **2018**, 20, 5559-5563	6.2	15
54	Screening and profiling stilbene-type natural products with angiotensin-converting enzyme inhibitory activity from Ampelopsis brevipedunculata var. hancei (Planch.) Rehder. *Journal of Pharmaceutical and Biomedical Analysis*, **2015**, 108, 70-7	3.5	14
53	Implementation of multiple-instance learning in drug activity prediction. *BMC Bioinformatics*, **2012**, 13 Suppl 15, S3	3.6	13
52	Intramolecular hydrogen bonds: ab initio Car-Parrinello simulations of arylamide torsions. *Chemical Physics Letters*, **2003**, 380, 150-157	2.5	13
51	Assignment of the absolute configuration of hepatoprotective highly oxygenated triterpenoids using X-ray, ECD, NMR J-based configurational analysis and HSQC overlay experiments. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 3089-3095	4	12

50	A novel natural phenyl alkene with cytotoxic activity. *Tetrahedron Letters*, **2013**, 54, 3872-3876	2	12
49	Imidazole-containing farnesyltransferase inhibitors: 3D quantitative structure-activity relationships and molecular docking. *Journal of Computer-Aided Molecular Design*, **2009**, 23, 431-48	4.2	12
48	Pharmacophore Modeling, Ensemble Docking, Virtual Screening, and Biological Evaluation on Glycogen Synthase Kinase-3 *Molecular Informatics*, **2014**, 33, 610-26	3.8	11
47	DFT study on the radical anions formed by primaquine and its derivatives. *Chemical Research in Toxicology*, **2011**, 24, 1476-85	4	11
46	Identification of a novel umami peptide in tempeh (Indonesian fermented soybean) and its binding mechanism to the umami receptor T1R. *Food Chemistry*, **2020**, 333, 127411	8.5	10
45	In silico investigation of lavandulyl flavonoids for the development of potent fatty acid synthase-inhibitory prototypes. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 3180-3188	4	10
44	Geometries and multipole moments of AlH4 SiH4, PH3, H2S and HCl. *Computational and Theoretical Chemistry*, **1999**, 488, 217-221		10
43	Semisynthetic latrunculin B analogs: studies of actin docking support a proposed mechanism for latrunculin bioactivity. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 7517-22	3.4	9
42	Quantitative structure-activity relationships of imidazole-containing farnesyltransferase inhibitors using different chemometric methods. *Medicinal Chemistry*, **2013**, 9, 434-48	1.8	9
41	Interactions of endocannabinoid virodhamine and related analogs with human monoamine oxidase-A and -B. *Biochemical Pharmacology*, **2018**, 155, 82-91	6	9
40	Puupehenone, a Marine-Sponge-Derived Sesquiterpene Quinone, Potentiates the Antifungal Drug Caspofungin by Disrupting Hsp90 Activity and the Cell Wall Integrity Pathway. *MSphere*, **2020**, 5,	5	8
39	Computationally assisted assignment of kahalalide Y configuration using an NMR-constrained conformational search. *Journal of Natural Products*, **2013**, 76, 178-85	4.9	8
38	Andrographolide induces apoptosis via down-regulation of glyoxalase 1 and HMG-CoA reductase in HL-60 cells. *Journal of Functional Foods*, **2015**, 14, 226-235	5.1	8
37	Structure-Based Identification of Potent Natural Product Chemotypes as Cannabinoid Receptor 1 Inverse Agonists. *Molecules*, **2018**, 23,	4.8	8
36	Quantitative Structure-Activity Relationship Analysis and a Combined Ligand-Based/Structure-Based Virtual Screening Study for Glycogen Synthase Kinase-3. *Molecular Informatics*, **2014**, 33, 627-40	3.8	7
35	Assignment of absolute configuration of sulfinyl dilactones: Optical rotations and 1H NMR experiment and DFT calculations. *Journal of Molecular Structure*, **2011**, 987, 166-173	3.4	7
34	Computational Study on the Conformations of Mitragynine and Mitragynaline. *Computational and Theoretical Chemistry*, **2010**, 945, 57-63		7
33	Structural and kinetic analyses of holothurian sulfated glycans suggest potential treatment for SARS-CoV-2 infection. *Journal of Biological Chemistry*, **2021**, 297, 101207	5.4	7

32	Salvindolin elicits opioid system-mediated antinociceptive and antidepressant-like activities. *Journal of Psychopharmacology*, **2019**, 33, 865-881	4.6	6
31	Agonists of the □aminobutyric acid type B (GABA) receptor derived from □hydroxy and □amino difluoromethyl ketones. *Bioorganic and Medicinal Chemistry Letters*, **2018**, 28, 2697-2700	2.9	6
30	Quinone propionic acid-based redox-triggered polymer nanoparticles for drug delivery: Computational analysis and in vitro evaluation. *Journal of Applied Polymer Science*, **2014**, 131, n/a-n/a	2.9	6
29	Asphodosides A-E, anti-MRSA metabolites from Asphodelus microcarpus. *Phytochemistry*, **2014**, 105, 79-84	4	6
28	Isolation and characterization of new secondary metabolites from. *Medicinal Chemistry Research*, **2014**, 23, 3510-3515	2.2	6
27	Structure of the cannabinoid receptor 1: homology modeling of its inactive state and enrichment study based on CB1 antagonist docking. *MedChemComm*, **2014**, 5, 1297-1302	5	6
26	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. *Chemical Research in Toxicology*, **2015**, 28, 169-74	4	6
25	Effect of antimalarial drug primaquine and its derivatives on the ionization potential of hemoglobin: A QM/MM study. *MedChemComm*, **2013**, 4, 1145-1147	5	6
24	Methemoglobin generation by 8-aminoquinolines: effect of substitution at 5-position of primaquine. *Chemical Research in Toxicology*, **2013**, 26, 1801-9	4	6
23	Optimization of sulfobutyl-ether-□cyclodextrin levels in oral formulations to enhance progesterone bioavailability. *International Journal of Pharmaceutics*, **2021**, 596, 120212	6.5	6
22	Hepatoprotective Tetrahydrobenzocyclooctabenzofuranone Lignans from. *Journal of Natural Products*, **2019**, 82, 2842-2851	4.9	5
21	Configurational assignments of conformationally restricted bis-monoterpene hydroquinones: utility in exploration of endangered plants. *Biochimica Et Biophysica Acta - General Subjects*, **2013**, 1830, 4229-34	4	5
20	Selective Interactions of -Methylated Flavonoid Natural Products with Human Monoamine Oxidase-A and -B. *Molecules*, **2020**, 25,	4.8	5
19	Antileishmanial Carbasugars from Geosmithia langdonii. *Journal of Natural Products*, **2018**, 81, 2222-2227	4.9	5
18	Hypervalent Iodine Mediated Oxidative Cyclization of Acrylamide -Carbamates to 5,5-Disubstituted Oxazolidine-2,4-diones. *Journal of Organic Chemistry*, **2020**, 85, 7549-7557	4.2	4
17	Multi-class Joint Rule Extraction and Feature Selection for Biological Data **2011**,		4
16	New Drugs from Natural Products around the World **2016**, 22, 215-216		4
15	Conformational properties of l-fucose and the tetrasaccharide building block of the sulfated l-fucan from Lytechinus variegatus. *Journal of Structural Biology*, **2020**, 209, 107407	3.4	4

14	Hydroxylated derivatives of NPC1161: theoretical insights into their potential toxicity and the feasibility and regioselectivity of their formation. *Journal of Physical Chemistry A*, **2014**, 118, 5501-7	2.8	3
13	Three-dimensional quantitative structure-farnesyltransferase inhibition analysis for some diaminobenzophenones. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2009**, 24, 1220-8	5.6	3
12	Are polarizabilities useful as aromaticity indices? Tests on azines, azoles, oxazoles and thiazoles. *Journal of Computational Methods in Sciences and Engineering*, **2004**, 4, 427-438	0.3	3
11	Methemoglobinemia Hemotoxicity of Some Antimalarial 8-Aminoquinoline Analogues and Their Hydroxylated Derivatives: Density Functional Theory Computation of Ionization Potentials. *Chemical Research in Toxicology*, **2016**, 29, 1132-41	4	2
10	Potential Modulation of Human NAD[P]H-Quinone Oxidoreductase 1 (NQO1) by EGCG and Its Metabolites-A Systematic Computational Study. *Chemical Research in Toxicology*, **2020**, 33, 2749-2764	4	2
9	Enantioselective Interactions of Anti-Infective 8-Aminoquinoline Therapeutics with Human Monoamine Oxidases A and B. *Pharmaceuticals*, **2021**, 14,	5.2	2
8	Negative allosteric modulators of cannabinoid receptor 1: Ternary complexes including CB1, orthosteric CP55940 and allosteric ORG27569. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-19	3.6	2
7	Data in support of optimized production of angiotensin-I converting enzyme inhibitory peptides derived from proteolytic hydrolysate of bitter melon seed proteins. *Data in Brief*, **2015**, 5, 403-7	1.2	1
6	Computational Study on the Conformations of Gambogic Acid. *Chemical Physics Letters*, **2011**, 511, 405-413	2.3	1
5	Cover Picture: Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers (Angew. Chem. Int. Ed. 9/2004). *Angewandte Chemie - International Edition*, **2004**, 43, 1033-1033	16.4	1
4	Fractionation of sulfated galactan from the red alga Botryocladia occidentalis separates its anticoagulant and anti-SARS-CoV-2 properties.. *Journal of Biological Chemistry*, **2022**, 101856	5.4	1
3	Validated determination of NRG1 Ig-like domain structure by mass spectrometry coupled with computational modeling.. *Communications Biology*, **2022**, 5, 452	6.7	1
2	Leveraging domain information to restructure biological prediction. *BMC Bioinformatics*, **2011**, 12 Suppl 10, S22	3.6	0
1	Titelbild: Nontoxic Membrane-Active Antimicrobial Arylamide Oligomers (Angew. Chem. 9/2004). *Angewandte Chemie*, **2004**, 116, 1051-1051	3.6	