

# Douglas B Kitchen

## List of Publications by Year in descending order

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43  
papers

4,347  
citations

279487

23  
h-index

264894

42  
g-index

44  
all docs

44  
docs citations

44  
times ranked

5640  
citing authors

#	ARTICLE	IF	CITATIONS
1	Docking and scoring in virtual screening for drug discovery: methods and applications. <i>Nature Reviews Drug Discovery</i> , 2004, 3, 935-949.	21.5	2,697
2	Gaussian fluctuation formula for electrostatic free energy changes in solution. <i>Journal of Chemical Physics</i> , 1991, 95, 3627-3633.	1.2	176
3	Molecular dynamics simulation of solvated protein at high pressure. <i>Biochemistry</i> , 1992, 31, 10083-10093.	1.2	144
4	Properly Oriented Heparin Decasaccharide-Induced Dimers Are the Biologically Active Form of Basic Fibroblast Growth Factor. <i>Biochemistry</i> , 1997, 36, 4782-4791.	1.2	111
5	Irreversible inhibition of epidermal growth factor receptor tyrosine kinase with In Vivo activity by N-[4-[(3-bromophenyl)amino]-6-quinazoliny]-2-butynamide (CL-387,785). <i>Biochemical Pharmacology</i> , 1999, 57, 917-925.	2.0	96
6	Molecular dynamics simulation of time-resolved fluorescence and nonequilibrium solvation of formaldehyde in water. <i>The Journal of Physical Chemistry</i> , 1990, 94, 4470-4476.	2.9	91
7	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. <i>Journal of Computational Chemistry</i> , 1990, 11, 1169-1180.	1.5	86
8	Organosilicon rings: structures and strain energies. <i>Journal of the American Chemical Society</i> , 1990, 112, 3408-3414.	6.6	80
9	Determining local conformational variations in DNA. <i>Journal of Molecular Biology</i> , 1990, 214, 711-736.	2.0	77
10	Computational models to predict blood-brain barrier permeation and CNS activity. <i>Journal of Computer-Aided Molecular Design</i> , 2003, 17, 643-664.	1.3	69
11	Early phase drug discovery: Cheminformatics and computational techniques in identifying lead series. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 5324-5342.	1.4	65
12	Solution structures of proteins from NMR data and modeling: alternative folds for neutrophil peptide 5. <i>Biochemistry</i> , 1989, 28, 9361-9372.	1.2	47
13	Design, Synthesis, and Evaluation of Nonretinoid Retinol Binding Protein 4 Antagonists for the Potential Treatment of Atrophic Age-Related Macular Degeneration and Stargardt Disease. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 7731-7757.	2.9	40
14	Median Partitioning: A Novel Method for the Selection of Representative Subsets from Large Compound Pools. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 885-893.	2.8	33
15	Design and Characterization of Novel Covalent Bromodomain and Extra-Terminal Domain (BET) Inhibitors Targeting a Methionine. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 8202-8211.	2.9	32
16	Determination of Protein Structures in Solution Using Nmr Data and Impact. <i>The International Journal of Supercomputer Applications</i> , 1988, 2, 41-61.	0.6	31
17	The design and synthesis of novel SGLT2 inhibitors: C-glycosides with benzyltriazolopyridinone and phenylhydantoin as the aglycone moieties. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 3414-3422.	1.4	31
18	A molecular dynamics study of pressure effects on solvation and optical spectra: the ground and excited states of formaldehyde in water. <i>The Journal of Physical Chemistry</i> , 1991, 95, 1082-1089.	2.9	30

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19	Computational approaches for modeling human intestinal absorption and permeability. <i>Journal of Molecular Modeling</i> , 2006, 12, 577-589.	0.8	29
20	Design and synthesis of aryl ether and sulfone hydroxamic acids as potent histone deacetylase (HDAC) inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 324-328.	1.0	26
21	Molecular Modeling of the Aldose Reductase-Inhibitor Complex Based on the X-ray Crystal Structure and Studies with Single-Site-Directed Mutants. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 1062-1070.	2.9	25
22	Bicyclic [3.3.0]-Octahydrocyclopenta[ <i>c</i> ]pyrrolo Antagonists of Retinol Binding Protein 4: Potential Treatment of Atrophic Age-Related Macular Degeneration and Stargardt Disease. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 5863-5888.	2.9	25
23	Lead Optimization toward Proof-of-Concept Tools for Huntington's Disease within a 4-(1H-Pyrazol-4-yl)pyrimidine Class of Pan-JNK Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 2967-2987.	2.9	24
24	Water binding in cryogenic liquids: The H <sub>2</sub> O...N <sub>2</sub> hydrogen bond. <i>Chemical Physics Letters</i> , 1987, 141, 525-529.	1.2	23
25	Zinc complexes of water, hydroxide, and ammonia. <i>The Journal of Physical Chemistry</i> , 1989, 93, 7265-7269.	2.9	22
26	4-Phenyl tetrahydroisoquinolines as dual norepinephrine and dopamine reuptake inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 7219-7222.	1.0	20
27	Discovery of a new chemical series of BRD4(1) inhibitors using protein-ligand docking and structure-guided design. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 2818-2823.	1.0	20
28	Systems biology-guided identification of synthetic lethal gene pairs and its potential use to discover antibiotic combinations. <i>Scientific Reports</i> , 2015, 5, 16025.	1.6	19
29	Discovery of Small-Molecule Antibiotics against a Unique tRNA-Mediated Regulation of Transcription in Gram-Positive Bacteria. <i>ChemMedChem</i> , 2019, 14, 758-769.	1.6	19
30	Design, Synthesis, and Preclinical Efficacy of Novel Nonretinoid Antagonists of Retinol-Binding Protein 4 in the Mouse Model of Hepatic Steatosis. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 5470-5500.	2.9	19
31	Solvent effects on the adiabatic free energy difference between the ground and excited states of methylindole in water. <i>The Journal of Physical Chemistry</i> , 1991, 95, 6756-6758.	2.9	18
32	Molecular structure calculations in two classes of conducting polymers. <i>Macromolecules</i> , 1983, 16, 190-192.	2.2	17
33	5-Functionalized indazoles as glucocorticoid receptor agonists. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 3017-3020.	1.0	17
34	The Anticancer Plant Triterpenoid, Avicin D, Regulates Glucocorticoid Receptor Signaling: Implications for Cellular Metabolism. <i>PLoS ONE</i> , 2011, 6, e28037.	1.1	17
35	Design, Selection, and Evaluation of a General Kinase-Focused Library. <i>ChemMedChem</i> , 2009, 4, 1273-1278.	1.6	16
36	Stabilization of $\beta$ -helical secondary structure during high-temperature molecular-dynamics simulations of $\beta$ -lactalbumin. <i>Chemical Physics</i> , 1991, 158, 295-301.	0.9	15

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37	Homology Model for Oncostatin M Based on NMR Structural Data. <i>Biochemistry</i> , 1998, 37, 10581-10588.	1.2	9
38	Computer-aided drug discovery research at a global contract research organization. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 309-318.	1.3	9
39	Model-driven discovery of synergistic inhibitors against <i>E. coli</i> and <i>S. enterica</i> serovar Typhimurium targeting a novel synthetic lethal pair, <i>aldA</i> and <i>prpC</i> . <i>Frontiers in Microbiology</i> , 2015, 6, 958.	1.5	8
40	Properly Oriented HeparinâDecasaccharide-Induced Dimers Are the Biologically Active Form of Basic Fibroblast Growth Factor. <i>Biochemistry</i> , 1997, 36, 7936-7936.	1.2	5
41	Design and Synthesis of 3-Arylisoxazoline-5-Carboxamide and 3-Arylisoxazoline-5-Acetamide Libraries as Potential Factor Xa Inhibitors. <i>Letters in Drug Design and Discovery</i> , 2012, 9, 2-7.	0.4	3
42	Simulating the effect of the two-spin approximation on the generation of protein structures from NOE data. <i>Journal of Magnetic Resonance</i> , 1992, 97, 398-410.	0.5	2
43	Median Partitioning: A Novel Method for the Selection of Representative Subsets from Large Compound Pools.. <i>ChemInform</i> , 2002, 33, 237-237.	0.1	0