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	Discovery of Smallâ€Molecule Antibiotics against a Unique tRNAâ€Mediated Regulation of Transcription in Gramâ€Positive Bacteria. ChemMedChem, 2019, 14, 758-769.	1.6	19
2	Design, Synthesis, and Preclinical Efficacy of Novel Nonretinoid Antagonists of Retinol-Binding Protein 4 in the Mouse Model of Hepatic Steatosis. Journal of Medicinal Chemistry, 2019, 62, 5470-5500.	2.9	19
3	Design and Characterization of Novel Covalent Bromodomain and Extra-Terminal Domain (BET) Inhibitors Targeting a Methionine. Journal of Medicinal Chemistry, 2018, 61, 8202-8211.	2.9	32
4	Computer-aided drug discovery research at a global contract research organization. Journal of Computer-Aided Molecular Design, 2017, 31, 309-318.	1.3	9
5	Systems biology-guided identification of synthetic lethal gene pairs and its potential use to discover antibiotic combinations. Scientific Reports, 2015, 5, 16025.	1.6	19
6	Model-driven discovery of synergistic inhibitors against E. coli and S. enterica serovar Typhimurium targeting a novel synthetic lethal pair, aldA and prpC. Frontiers in Microbiology, 2015, 6, 958.	1.5	8
7	Lead Optimization toward Proof-of-Concept Tools for Huntingtonâ€™s Disease within a 4-(1H-Pyrazol-4-yl)pyrimidine Class of Pan-JNK Inhibitors. Journal of Medicinal Chemistry, 2015, 58, 2967-2987.	2.9	24
8	Bicyclic [3.3.0]-Octahydrocyclopenta[c]pyrrolo Antagonists of Retinol Binding Protein 4: Potential Treatment of Atrophic Age-Related Macular Degeneration and Stargardt Disease. Journal of Medicinal Chemistry, 2015, 58, 5863-5888.	2.9	25
9	Discovery of a new chemical series of BRD4(1) inhibitors using protein-ligand docking and structure-guided design. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 2818-2823.	1.0	20
10	The design and synthesis of novel SGLT2 inhibitors: C-glycosides with benzyltriazolopyridinone and phenylhydantoin as the aglycone moieties. Bioorganic and Medicinal Chemistry, 2014, 22, 3414-3422.	1.4	31
11	Design, Synthesis, and Evaluation of Nonretinoid Retinol Binding Protein 4 Antagonists for the Potential Treatment of Atrophic Age-Related Macular Degeneration and Stargardt Disease. Journal of Medicinal Chemistry, 2014, 57, 7731-7757.	2.9	40
12	Design and Synthesis of 3-Arylisoxazoline-5-Carboxamide and 3-Arylisoxazoline-5-Acetamide Libraries as Potential Factor Xa Inhibitors. Letters in Drug Design and Discovery, 2012, 9, 2-7.	0.4	3
13	4-Phenyl tetrahydroisoquinolines as dual norepinephrine and dopamine reuptake inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 7219-7222.	1.0	20
14	Early phase drug discovery: Cheminformatics and computational techniques in identifying lead series. Bioorganic and Medicinal Chemistry, 2012, 20, 5324-5342.	1.4	65
15	The Anticancer Plant Triterpenoid, Avicin D, Regulates Glucocorticoid Receptor Signaling: Implications for Cellular Metabolism. PLoS ONE, 2011, 6, e28037.	1.1	17
16	Design and synthesis of aryl ether and sulfone hydroxamic acids as potent histone deacetylase (HDAC) inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 324-328.	1.0	26
17	5-Functionalized indazoles as glucocorticoid receptor agonists. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 3017-3020.	1.0	17
18	Design, Selection, and Evaluation of a General Kinaseâ€Focused Library. ChemMedChem, 2009, 4, 1273-1278.	1.6	16

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19	Computational approaches for modeling human intestinal absorption and permeability. Journal of Molecular Modeling, 2006, 12, 577-589.	0.8	29
20	Docking and scoring in virtual screening for drug discovery: methods and applications. Nature Reviews Drug Discovery, 2004, 3, 935-949.	21.5	2,697
21	Computational models to predict bloodâ€“brain barrier permeation and CNS activity. Journal of Computer-Aided Molecular Design, 2003, 17, 643-664.	1.3	69
22	Median Partitioning:â€‰ A Novel Method for the Selection of Representative Subsets from Large Compound Pools. Journal of Chemical Information and Computer Sciences, 2002, 42, 885-893.	2.8	33
23	Median Partitioning: A Novel Method for the Selection of Representative Subsets from Large Compound Pools.. ChemInform, 2002, 33, 237-237.	0.1	0
24	Molecular Modeling of the Aldose Reductase-Inhibitor Complex Based on the X-ray Crystal Structure and Studies with Single-Site-Directed Mutants. Journal of Medicinal Chemistry, 2000, 43, 1062-1070.	2.9	25
25	Irreversible inhibition of epidermal growth factor receptor tyrosine kinase with In Vivo activity by N-[4-[(3-bromophenyl)amino]-6-quinazolinyl]-2-butynamide (CL-387,785). Biochemical Pharmacology, 1999, 57, 917-925.	2.0	96
26	Homology Model for Oncostatin M Based on NMR Structural Data. Biochemistry, 1998, 37, 10581-10588.	1.2	9
27	Properly Oriented Heparinâ^'Decasaccharide-Induced Dimers Are the Biologically Active Form of Basic Fibroblast Growth Factorâ€‚â€¡. Biochemistry, 1997, 36, 4782-4791.	1.2	111
28	Properly Oriented Heparinâ^'Decasaccharide-Induced Dimers Are the Biologically Active Form of Basic Fibroblast Growth Factor. Biochemistry, 1997, 36, 7936-7936.	1.2	5
29	Molecular dynamics simulation of solvated protein at high pressure. Biochemistry, 1992, 31, 10083-10093.	1.2	144
30	Simulating the effect of the two-spin approximation on the generation of protein structures from NOE data. Journal of Magnetic Resonance, 1992, 97, 398-410.	0.5	2
31	A molecular dynamics study of pressure effects on solvation and optical spectra: the ground and excited states of formaldehyde in water. The Journal of Physical Chemistry, 1991, 95, 1082-1089.	2.9	30
32	Solvent effects on the adiabatic free energy difference between the ground and excited states of methylindole in water. The Journal of Physical Chemistry, 1991, 95, 6756-6758.	2.9	18
33	Stabilization of Î±-helical secondary structure during high-temperature molecular-dynamics simulations of Î±-lactalbumin. Chemical Physics, 1991, 158, 295-301.	0.9	15
34	Gaussian fluctuation formula for electrostatic freeâ€energy changes in solution. Journal of Chemical Physics, 1991, 95, 3627-3633.	1.2	176
35	Conserving energy during molecular dynamics simulations of water, proteins, and proteins in water. Journal of Computational Chemistry, 1990, 11, 1169-1180.	1.5	86
36	Molecular dynamics simulation of time-resolved fluorescence and nonequilibrium solvation of formaldehyde in water. The Journal of Physical Chemistry, 1990, 94, 4470-4476.	2.9	91

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37	Organosilicon rings: structures and strain energies. Journal of the American Chemical Society, 1990, 112, 3408-3414.	6.6	80
38	Determining local conformational variations in DNA. Journal of Molecular Biology, 1990, 214, 711-736.	2.0	77
39	Zinc complexes of water, hydroxide, and ammonia. The Journal of Physical Chemistry, 1989, 93, 7265-7269.	2.9	22
40	Solution structures of proteins from NMR data and modeling: alternative folds for neutrophil peptide 5. Biochemistry, 1989, 28, 9361-9372.	1.2	47
41	Determination of Protein Structures in Solution Using Nmr Data and Impact. The International Journal of Supercomputer Applications, 1988, 2, 41-61.	0.6	31
42	Water binding in cryogenic liquids: The H2Oâ€¦N2 hydrogen bond. Chemical Physics Letters, 1987, 141, 525-529.	1.2	23
43	Molecular structure calculations in two classes of conducting polymers. Macromolecules, 1983, 16, 190-192.	2.2	17