Gerald Henry Lushington

List of Publications by Year
in descending order

175	4,193	101496	161767
papers	citations	36 h-index	54 g-index

185	185	185	5361
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Utilization of Hydrogen Bonds To Stabilize Mâ"O(H) Units:â€‰ Synthesis and Properties of Monomeric Iron and Manganese Complexes with Terminal Oxo and Hydroxo Ligands. Journal of the American Chemical Society, 2004, 126, 2556-2567.	6.6	173
2	Novel splice isoforms for NLGN3 and NLGN4 with possible implications in autism. Journal of Medical Genetics, 2005, 43, e21-e21.	1.5	148
3	How the mutation glycine96 to alanine confers glyphosate insensitivity to 5-enolpyruvyl shikimate-3-phosphate synthase from Escherichia coli. Planta, 2002, 216, 129-135.	1.6	98
4	Structure-guided design of potent and permeable inhibitors of MERS coronavirus 3CL protease that utilize a piperidine moiety as a novel design element. European Journal of Medicinal Chemistry, 2018, 150, 334-346.	2.6	96
5	Orientational Dynamics and Dye-DNA Interactions in a Dye-Labeled DNA Aptamer. Biophysical Journal, 2005, 88, 3455-3465.	0.2	94
6	Differential Inhibition of Adenylyl Cyclase Isoforms and Soluble Guanylyl Cyclase by Purine and Pyrimidine Nucleotides. Journal of Biological Chemistry, 2004, 279, 19955-19969.	1.6	91
7	Structure of the Human Lung Cytochrome P450 2A13. Journal of Biological Chemistry, 2007, 282, 17306-17313.	1.6	90
8	Inhibitors of membranous adenylyl cyclases. Trends in Pharmacological Sciences, 2012, 33, 64-78.	4.0	90
9	Activation and Inhibition of Adenylyl Cyclase Isoforms by Forskolin Analogs. Journal of Pharmacology and Experimental Therapeutics, 2008, 325, 27-36.	1.3	81
10	Deoxycholate Interacts with IpaD of Shigella flexneri in Inducing the Recruitment of IpaB to the Type III Secretion Apparatus Needle Tip. Journal of Biological Chemistry, 2008, 283, 18646-18654.	1.6	79
11	Ab initio study of molecularg-tensors. International Journal of Quantum Chemistry, 1995, 55, 377-392.	1.0	71
12	Solution Phase Synthesis of a Diverse Library of Highly Substituted Isoxazoles. ACS Combinatorial Science, 2008, 10, 658-663.	3.3	67
13	Inhibition of Dengue virus and West Nile virus proteases by click chemistry-derived benz[d]isothiazol-3(2H)-one derivatives. Bioorganic and Medicinal Chemistry, 2012, 20, 1213-1221.	1.4	67
14	Discovery and Structural Modification of Inhibitors of Methionine Aminopeptidases from Escherichia coli and Saccharomyces cerevisiae. Journal of Medicinal Chemistry, 2003, 46, 2631-2640.	2.9	66
15	Canine cathelicidin (K9CATH): Gene cloning, expression, and biochemical activity of a novel pro-myeloid antimicrobial peptide. Developmental and Comparative Immunology, 2007, 31, 1278-1296.	1.0	66
16	Design, synthesis and characterization of novel 1,2-benzisothiazol-3(2H)-one and 1,3,4-oxadiazole hybrid derivatives: Potent inhibitors of Dengue and West Nile virus NS2B/NS3 proteases. Bioorganic and Medicinal Chemistry, 2013, 21, 102-113.	1.4	60
17	Parallel Synthesis of a Multi-Substituted Benzo[b]furan Library. ACS Combinatorial Science, 2008, 10, 941-947.	3.3	59
18	Comprehensive Study of Sansalvamide A Derivatives and their Structureâ€"Activity Relationships against Drug-Resistant Colon Cancer Cell Lines. Journal of Medicinal Chemistry, 2008, 51, 530-544.	2.9	55

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19	Solution-Phase Parallel Synthesis of a Multi-substituted Benzo[b]thiophene Library. ACS Combinatorial Science, 2009, 11, 900-906.	3.3	55
20	Solution-Phase Parallel Synthesis of a Diverse Library of 1,2-Dihydroisoquinolines. ACS Combinatorial Science, 2011, 13, 265-271.	3.8	54
21	Potent inhibition of norovirus 3CL protease by peptidyl Î±-ketoamides and Î±-ketoheterocycles. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 4820-4826.	1.0	54
22	Encircled Proton. Journal of the American Chemical Society, 2007, 129, 8692-8693.	6.6	51
23	A Docking Score Function for Estimating Ligandâ"Protein Interactions:â€‰ Application to Acetylcholinesterase Inhibition. Journal of Medicinal Chemistry, 2004, 47, 5492-5500.	2.9	49
24	Uptake, Distribution and Diffusivity of Reactive Fluorophores in Cells: Implications toward Target Identification. Molecular Pharmaceutics, 2010, 7, 1301-1310.	2.3	49
25	LipidomeDB Data Calculation Environment: Online Processing of Directâ€Infusion Mass Spectral Data for Lipid Profiles. Lipids, 2011, 46, 879-884.	0.7	49
26	Mechanistic Insight into Acetylcholinesterase Inhibition and Acute Toxicity of Organophosphorus Compounds:Â A Molecular Modeling Study. Chemical Research in Toxicology, 2006, 19, 209-216.	1.7	48
27	Design, synthesis, and evaluation of inhibitors of Norwalk virus 3C protease. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5315-5319.	1.0	46
28	One-Step Synthesis of Oxazoline and Dihydrooxazine Libraries. ACS Combinatorial Science, 2007, 9, 473-476.	3.3	45
29	A filter-based feature selection approach for identifying potential biomarkers for lung cancer. Journal of Clinical Bioinformatics, 2011, 1, 11.	1.2	45
30	Inhibitors of Dengue virus and West Nile virus proteases based on the aminobenzamide scaffold. Bioorganic and Medicinal Chemistry, 2012, 20, 4140-4148.	1.4	43
31	Key Residues Controlling Binding of Diverse Ligands to Human Cytochrome P450 2A Enzymes. Drug Metabolism and Disposition, 2009, 37, 1319-1327.	1.7	40
32	Reagent based DOS: A â€œClick, Click, Cyclizeâ€•strategy to probe chemical space. Organic and Biomolecular Chemistry, 2010, 8, 2198.	1.5	40
33	Synthesis of a Unique Isoindoline/Tetrahydroisoquinoline-based Tricyclic Sultam Library Utilizing a Heck-aza-Michael Strategy. ACS Combinatorial Science, 2012, 14, 211-217.	3.8	40
34	Macrocyclic inhibitors of 3C and 3C-like proteases of picornavirus, norovirus, and coronavirus. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 3709-3712.	1.0	40
35	Glycosylation Effects on FSH-FSHR Interaction Dynamics: A Case Study of Different FSH Glycoforms by Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0137897.	1.1	40
36	Modular Synthesis of Cyclic Peptidomimetics Inspired by Î³-Turnsâ€. Organic Letters, 2005, 7, 1059-1062.	2.4	37

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37	Whither Combine? New Opportunities for Receptor-Based QSAR. Current Medicinal Chemistry, 2007, 14, 1863-1877.	1.2	37
38	Identification, Ki determination and CoMFA analysis of nuclear receptor ligands as competitive inhibitors of OATP1B1-mediated estradiol-17Î²-glucuronide transport. Pharmacological Research, 2009, 60, 50-56.	3.1	35
39	Organometallic Isocyanocyclopentadienides:Â A Combined Synthetic, Spectroscopic, Structural, Electrochemical, and Theoretical Investigation. Organometallics, 2004, 23, 2927-2938.	1.1	34
40	Interaction of Phosphonate Analogues of the Tetrahedral Reaction Intermediate with 5-Enolpyruvylshikimate-3-phosphate Synthase in Atomic Detailâ€,â€¡. Biochemistry, 2005, 44, 3241-3248.	1.2	33
41	Design, synthesis, and antiproliferative and CDK2-cyclin a inhibitory activity of novel flavopiridol analogues. Bioorganic and Medicinal Chemistry, 2007, 15, 702-713.	1.4	33
42	Solution-Phase Synthesis of a Highly Substituted Furan Library. ACS Combinatorial Science, 2012, 14, 403-414.	3.8	33
43	The electronicg-tensor of MgF: A comparison of ROHF and MRD?CI level results. International Journal of Quantum Chemistry, 1996, 60, 1679-1684.	1.0	32
44	Theoretically predicted structures of plasma membrane Ca2+-ATPase and their susceptibilities to oxidation. Journal of Molecular Graphics and Modelling, 2005, 24, 175-185.	1.3	32
45	Application of 6,7-Indole Aryne Cycloaddition and Pd(0)-Catalyzed Suzukiâ€“Miyaura and Buchwaldâ€“Hartwig Cross-Coupling Reactions for the Preparation of Annulated Indole Libraries. ACS Combinatorial Science, 2011, 13, 443-448.	3.8	32
46	1,3â€Allylic Strain as a Strategic Diversification Element for Constructing Libraries of Substituted 2â€Arylpiperidines. Angewandte Chemie - International Edition, 2011, 50, 2734-2737.	7.2	32
47	Stability, properties and electronic g-tensors of H2COâ¯ as stabilized in H2COÂ·Na complexes. Chemical Physics, 1997, 225, 1-15.	0.9	31
48	First Homoleptic Complexes of Isocyanoferrocene. Journal of the American Chemical Society, 2002, 124, 13668-13669.	6.6	31
49	A Modular Reaction Pairing Approach to the Diversity-Oriented Synthesis of Fused- and Bridged-Polycyclic Sultams. Organic Letters, 2011, 13, 5148-5151.	2.4	31
50	Structure-based design and synthesis of triazole-based macrocyclic inhibitors of norovirus protease: Structural, biochemical, spectroscopic, and antiviral studies. European Journal of Medicinal Chemistry, 2016, 119, 300-318.	2.6	30
51	Small Closed-Form CI Expansions for Electronic g-Tensor Calculations. Journal of Physical Chemistry A, 2000, 104, 2969-2974.	1.1	29
52	Temperature dependent 2nd derivative absorbance spectroscopy of aromatic amino acids as a probe of protein dynamics. Protein Science, 2009, 18, 2603-2614.	3.1	29
53	One-Pot, Three-Component, Domino Heck-aza-Michael Approach to Libraries of Functionalized 1,1-Dioxido-1,2-benzisothiazoline-3-acetic Acids. ACS Combinatorial Science, 2009, 11, 732-738.	3.3	28
54	G-hash. , 2009, 360, 472-480.		27

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55	Targeting of Histone Acetyltransferase p300 by Cyclopentenone Prostaglandin Î”¹²-PGJ₂ through Covalent Binding to Cys¹⁴³⁸. Chemical Research in Toxicology, 2012, 25, 337-347.	1.7	27
56	Design, Synthesis, and In Vitro Evaluation of Potential West Nile Virus Protease Inhibitors Based on the 1-Oxo-1,2,3,4-tetrahydroisoquinoline and 1-Oxo-1,2-dihydroisoquinoline Scaffolds. ACS Combinatorial Science, 2010, 12, 836-843.	3.3	26
57	Quantum mechanics and mixed quantum mechanics/molecular mechanics simulations of model nerve agents with acetylcholinesterase. Theoretical Chemistry Accounts, 2003, 109, 160-168.	0.5	25
58	GPM: A graph pattern matching kernel with diffusion for chemical compound classification. , 2008, 2008, 1-6.		25
59	GRAPH WAVELET ALIGNMENT KERNELS FOR DRUG VIRTUAL SCREENING. Journal of Bioinformatics and Computational Biology, 2009, 07, 473-497.	0.3	25
60	Highly Substituted Indole Library Synthesis by Palladium-Catalyzed Coupling Reactions in Solution and on a Solid Support. ACS Combinatorial Science, 2009, 11, 875-879.	3.3	25
61	Potent inhibition of norovirus by dipeptidyl Î±-hydroxyphosphonate transition state mimics. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5941-5944.	1.0	25
62	Solution-Phase Parallel Synthesis of a Library of Î”2-Pyrazolines. ACS Combinatorial Science, 2007, 9, 20-28.	3.3	24
63	Synthesis of an Isoindoline-Annulated, Tricyclic Sultam Library via Microwave-Assisted, Continuous-Flow Organic Synthesis (MACOS). Synthesis, 2012, 44, 2547-2554.	1.2	24
64	Oxadiazole-Based Cell Permeable Macrocyclic Transition State Inhibitors of Norovirus 3CL Protease. Journal of Medicinal Chemistry, 2016, 59, 1899-1913.	2.9	24
65	Five Possible Isocyanoazulenes and Electron-Rich Complexes Thereof:â€‰ A Quantitative Organometallic Approach for Probing Electronic Inhomogeneity of the Azulenic Framework. Organometallics, 2005, 24, 2386-2397.	1.1	23
66	Solution-Phase Synthesis of a Diverse Library of Benzisoxazoles Utilizing the [3 + 2] Cycloaddition of in Situ-Generated Nitrile Oxides and Arynes. ACS Combinatorial Science, 2013, 15, 193-201.	3.8	23
67	Electron-spin g-factors of H2â^'. An ab initio study. Chemical Physics Letters, 1996, 258, 427-430.	1.2	22
68	The 2,6-Diisocyanoazulene Motif:Â Synthesis and Efficient Mono- and Heterobimetallic Complexation with Controlled Orientation of the Azulenic Dipole. Journal of the American Chemical Society, 2006, 128, 2300-2309.	6.6	21
69	Acetylcholinesterase: Molecular Modeling with the Whole Toolkit. Current Topics in Medicinal Chemistry, 2006, 6, 57-73.	1.0	21
70	First Isocyanoazulene and Its Homoleptic Complexes. Journal of the American Chemical Society, 2003, 125, 4432-4433.	6.6	20
71	Discover protein sequence signatures from protein-protein interaction data. BMC Bioinformatics, 2005, 6, 277.	1.2	20
72	Utilization of the 1,2,3,5-thiatriazolidin-3-one 1,1-dioxide scaffold in the design of potential inhibitors of human neutrophil proteinase 3. Bioorganic and Medicinal Chemistry, 2010, 18, 1093-1102.	1.4	20

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73	S_NAr-Based, Facile Synthesis of a Library of Benzothiaoxazepine-1,1â€²-dioxides. ACS Combinatorial Science, 2010, 12, 850-854.	3.3	20
74	Facile (Triazolyl)methylation of MACOS-derived Benzofused Sultams Utilizing ROMP-derived OTP Reagents. ACS Combinatorial Science, 2012, 14, 268-272.	3.8	20
75	Structure-based exploration and exploitation of the S4 subsite of norovirus 3CL protease in the design of potent and permeable inhibitors. European Journal of Medicinal Chemistry, 2017, 126, 502-516.	2.6	20
76	Automated Synthesis of a 184-Member Library of Thiadiazepan-1,1-dioxide-4-ones. ACS Combinatorial Science, 2011, 13, 244-250.	3.8	19
77	Comparison of Thioethers and Sulfoxides as Axial Ligands forN-Acetylmicroperoxidase-8:Â Implications for Oxidation of Methionine-80 in Cytochromec. Inorganic Chemistry, 2003, 42, 7550-7559.	1.9	18
78	Novel synthetic inhibitors of 3-hydroxy-3-methylglutaryl-coenzyme A (HMG-CoA) reductase activity that inhibit tumor cell proliferation and are structurally unrelated to existing statins. International Journal of Molecular Medicine, 2009, 24, 633-43.	1.8	18
79	Mechanism-based inhibitors of serine proteases with high selectivity through optimization of Sâ€² subsite binding. Bioorganic and Medicinal Chemistry, 2009, 17, 3536-3542.	1.4	18
80	The major vault protein is related to the toxic anion resistance protein(TelA) family. Journal of Experimental Biology, 2007, 210, 946-955.	0.8	17
81	Structureâ€“activity relationships for the interactions of 2â€²- and 3â€²-(O)-(N-methyl)anthraniloyl-substituted purine and pyrimidine nucleotides with mammalian adenylyl cyclases. Biochemical Pharmacology, 2011, 82, 358-370.	2.0	17
82	Solution-Phase Parallel Synthesis of a Multisubstituted Cyclic Imidate Library. ACS Combinatorial Science, 2013, 15, 247-254.	3.8	17
83	Configuration interaction study of relativistic corrections to the zeeman effect in diatomic molecules. International Journal of Quantum Chemistry, 1995, 56, 283-288.	1.0	16
84	Differential interactions of G-proteins and adenylyl cyclase with nucleoside 5â€²-triphosphates, nucleoside 5â€²-[Î³-thio]triphosphates and nucleoside 5â€²-[Î²,Î³-imido]triphosphates. Biochemical Pharmacology, 2005, 71, 89-97.	2.0	16
85	Solution-Phase Parallel Synthesis of Hexahydro-1H-isoindolone Libraries via Tactical Combination of Cu-Catalyzed Three-Component Coupling and Dielsâ€“Alder Reactions. ACS Combinatorial Science, 2008, 10, 285-302.	3.3	16
86	Studies Towards the Synthesis of Methionine Aminopeptidase Inhibitors: Diversification Utilizing a ROMP-Derived Coupling Reagent. ACS Combinatorial Science, 2008, 10, 195-203.	3.3	16
87	Design and Synthesis of Medium-Ring Lactam Libraries Inspired by Octalactin A. A Convergentâ^'Divergent Approach. ACS Combinatorial Science, 2008, 10, 628-631.	3.3	16
88	Crystal Structure of Histamine Dehydrogenase from Nocardioides simplex. Journal of Biological Chemistry, 2010, 285, 25782-25791.	1.6	16
89	Ab Initio and Density Functional Study of the Electronic Transitions of Indoline and Indoline-2-Carboxylic Acid. Journal of Physical Chemistry A, 2003, 107, 5670-5680.	1.1	15
90	Differences in Paclitaxel and Docetaxel Interactions with Tubulin Detected by Mutagenesis of Yeast Tubulin. ChemMedChem, 2008, 3, 1844-1847.	1.6	15

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91	The BioAssay network and its implications to future therapeutic discovery. BMC Bioinformatics, 2011, 12, S1.	1.2	15
92	The 3q29 microdeletion syndrome: Report of three new unrelated patients and in silico â€œRNA bindingâ€• analysis of the 3q29 region. American Journal of Medical Genetics, Part A, 2011, 155, 1654-1660.	0.7	14
93	Automated Synthesis of a Library of Triazolated 1,2,5-Thiadiazepane 1,1-Dioxides via a Double Aza-Michael Strategy. ACS Combinatorial Science, 2012, 14, 456-459.	3.8	14
94	Stability and Electronic Properties of Nitrogen Nanoneedles and Nanotubes. Journal of Chemical Information and Modeling, 2006, 46, 1965-1971.	2.5	13
95	Support Vector Machines in HTS Data Mining: Type I MetAPs Inhibition Study. Journal of Biomolecular Screening, 2006, 11, 138-144.	2.6	13
96	Synthesis of Amino-Benzothiaoxazepine-1,1-dioxides Utilizing a Microwave-Assisted, S_NAr Protocol. ACS Combinatorial Science, 2011, 13, 653-658.	3.8	13
97	An Overview of Computational Life Science Databases & Exchange Formats of Relevance to Chemical Biology Research. Combinatorial Chemistry and High Throughput Screening, 2013, 16, 189-198.	0.6	13
98	Electron-spin magnetic moments of the2?+ ions Li2+, Li2?, and Be2+: An ab initio ROHF study. International Journal of Quantum Chemistry, 1997, 63, 511-521.	1.0	12
99	Molecular modeling analysis of the interaction of novel bis-cationic ligands with the lipid A moiety of lipopolysaccharide. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 714-717.	1.0	12
100	The paclitaxel site in tubulin probed by siteâ€directed mutagenesis of Saccharomyces cerevisiae Î²â€tubulin. FEBS Letters, 2008, 582, 2467-2470.	1.3	12
101	Characterizing the Diversity and Biological Relevance of the MLPCN Assay Manifold and Screening Set. Journal of Chemical Information and Modeling, 2011, 51, 1205-1215.	2.5	12
102	Design, synthesis, and evaluation of a novel series of macrocyclic inhibitors of norovirus 3CL protease. European Journal of Medicinal Chemistry, 2017, 127, 41-61.	2.6	12
103	Distinct interactions of 2â€²- and 3â€²-O-(N-methyl)anthraniloyl-isomers of ATP and GTP with the adenylyl cyclase toxin of Bacillus anthracis, edema factor. Biochemical Pharmacology, 2009, 78, 224-230.	2.0	11
104	Triazole-Containing Isothiazolidine 1,1-Dioxide Library Synthesis: One-Pot, Multi-Component Protocols for Small Molecular Probe Discovery. ACS Combinatorial Science, 2011, 13, 511-517.	3.8	11
105	Structural Basis for the High-Affinity Inhibition of Mammalian Membranous Adenylyl Cyclase by 2â€²,3â€²-O-(N-Methylanthraniloyl)-Inosine 5â€²-Triphosphate. Molecular Pharmacology, 2011, 80, 87-96.	1.0	11
106	Deamidation of model Î²-turn cyclic peptides in the solid state. Journal of Pharmaceutical Sciences, 2005, 94, 2616-2631.	1.6	10
107	A conformational transition in the adenylyl cyclase catalytic site yields different binding modes for ribosyl-modified and unmodified nucleotide inhibitors. Bioorganic and Medicinal Chemistry, 2007, 15, 2993-3002.	1.4	10
108	Ionic Immobilization, Diversification, and Release: Application to the Generation of a Library of Methionine Aminopeptidase Inhibitors. ACS Combinatorial Science, 2008, 10, 185-194.	3.3	10

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109	FEATURE SELECTION IN VALIDATING MASS SPECTROMETRY DATABASE SEARCH RESULTS. Journal of Bioinformatics and Computational Biology, 2008, 06, 223-240.	0.3	10
110	Feature Selection in the Tensor Product Feature Space. , 2009, , 1004-1009.		10
111	Structure-Guided Optimization of Dipeptidyl Inhibitors of Norovirus 3CL Protease. Journal of Medicinal Chemistry, 2020, 63, 11945-11963.	2.9	10
112	Monte Carlo simulations of CO2-expanded acetonitrile. Molecular Physics, 2006, 104, 2955-2960.	0.8	9
113	Application of kernel functions for accurate similarity search in large chemical databases. BMC Bioinformatics, 2010, 11, S8.	1.2	9
114	Interactions of Bordetella pertussis adenylyl cyclase toxin CyaA with calmodulin mutants and calmodulin antagonists: Comparison with membranous adenylyl cyclase I. Biochemical Pharmacology, 2012, 83, 839-848.	2.0	9
115	Comparative Modeling of Proteins. Methods in Molecular Biology, 2015, 1215, 309-330.	0.4	9
116	Interactions of organophosphorus and related compounds with cholinesterases, a theoretical study. Chemico-Biological Interactions, 2005, 157-158, 321-325.	1.7	8
117	Structure-guided design, synthesis and evaluation of oxazolidinone-based inhibitors of norovirus 3CL protease. European Journal of Medicinal Chemistry, 2018, 143, 881-890.	2.6	8
118	Rat Cardiomyocytes Express a Classical Epithelial Beta-Defensin. American Journal of Animal and Veterinary Sciences, 2008, 3, 1-6.	0.2	8
119	Ab initio simulation of physisorption: N2 on pregraphitic clusters. Computational and Theoretical Chemistry, 2001, 544, 221-235.	1.5	7
120	GPD: A Graph Pattern Diffusion Kernel for Accurate Graph Classification with Applications in Cheminformatics. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2010, 7, 197-207.	1.9	7
121	Differentiating between Models of Epothilone Binding to Microtubules Using Tubulin Mutagenesis, Cytotoxicity, and Molecular Modeling. ChemMedChem, 2012, 7, 1580-1586.	1.6	7
122	Biomedical research: a house of cards?. Future Medicinal Chemistry, 2016, 8, 1-5.	1.1	7
123	The electron-spin magnetic moment (g-tensor) of H2CO+ according to MRCI calculations. Computational and Theoretical Chemistry, 2000, 527, 139-148.	1.5	6
124	Antitumor effects of synthetic 6,7-annulated-4-substituted indole compounds in L1210 leukemic cells in vitro. Anticancer Research, 2012, 32, 4671-84.	0.5	6
125	Comparative Modeling of Proteins. Methods in Molecular Biology, 2008, 443, 199-212.	0.4	5
126	CGM: A biomedical text categorization approach using concept graph mining. , 2009, , .		5

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127	Exploring chemical diversity via a modular reaction pairing strategy. Beilstein Journal of Organic Chemistry, 2012, 8, 1293-1302.	1.3	5
128	Protein Glycation: An Old Villain is Shedding Secrets. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 362-369.	0.6	5
129	Anti-Endotoxin Agents. 3. Rapid Identification of High-Affinity Lipopolysaccharide-Binding Compounds in a Substituted Polyamine Library. Combinatorial Chemistry and High Throughput Screening, 2006, 9, 27-36.	0.6	4
130	Structure-Based Quantitative Structure Activity Relationship Analysis of Omuralide Analogs in the 20S Proteasome: A Covalent Inhibitor COMBINE Study. Letters in Drug Design and Discovery, 2007, 4, 417-421.	0.4	4
131	Bioinformatics process management: information flow via a computational journal. Source Code for Biology and Medicine, 2007, 2, 9.	1.7	4
132	To screen or not to screen: an impassioned plea for smarter chemical libraries to improve drug lead finding. Future Medicinal Chemistry, 2014, 6, 497-502.	1.1	4
133	Meet Our Editor. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 1-1.	0.6	4
134	GRAPH WAVELET ALIGNMENT KERNELS FOR DRUG VIRTUAL SCREENING. , 2008, , .		4
135	Mechanisms by which synthetic 6,7-annulated-4-substituted indole compounds with anti-proliferative activity disrupt mitosis and block cytokinesis in human HL-60 tumor cells in vitro. Anticancer Research, 2014, 34, 1643-55.	0.5	4
136	Novel Algorithms for the Identification of Biologically Informative Chemical Diversity Metrics. Current Computer-Aided Drug Design, 2008, 4, 23-34.	0.8	3
137	The C1 homodimer of adenylyl cyclase binds nucleotides with high affinity but possesses exceedingly low catalytic activity. Neuroscience Letters, 2009, 467, 1-5.	1.0	3
138	Chemical Informatics and the Drug Discovery Knowledge Pyramid. Combinatorial Chemistry and High Throughput Screening, 2013, 16, 764-776.	0.6	3
139	Enantiospecific Synthesis and Cytotoxicity Evaluation of Oximidineâ€...II Analogues. ChemMedChem, 2016, 11, 1600-1616.	1.6	3
140	G-Hash. Advances in Data Mining and Database Management Book Series, 0, , 176-213.	0.4	3
141	CoMSIA/QSAR Models for Vacuolar (H+) ATPase Inhibition by Selected Benzoate and Benzolactone Species. Letters in Drug Design and Discovery, 2006, 3, 104-107.	0.4	2
142	Notice of Violation of IEEE Publication Principles - Systematically Identifying Genes and Pathways in Multiple Cancer Types Using HGD & PSO-SVM. , 2009, , .		2
143	Oncogenes and pathway identification using filter-based approaches between various carcinoma types in lung. International Journal of Computational Biology and Drug Design, 2009, 2, 236.	0.3	2
144	Chemistry, Screening, and the Democracy of Publishing. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 288-289.	0.6	2

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145	Perspective on the COVID-19 Coronavirus Outbreak. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 90-91.	0.6	2
146	GlycomicsDB - A Data Integration Platform for Glycans and their Strucutres. Open Medical Informatics Journal, 2011, 5, 9-17.	1.0	2
147	A multi-tier data mining workflow to analyze the age related shift from diglycosylated- to tetra-glycosylated-FSH secretion by the anterior pituitary. , 2010, , .		1
148	Multi-target protein-chemical interaction prediction using task-regularized and boosted multi-task learning. , 2012, , .		1
149	Editorial: Computational Toxicology: Screening, Chemistry, or Much More?. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 733-733.	0.6	1
150	Editorial: Mining for Pharmacophores in Phenotypic Screens. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 651-651.	0.6	1
151	Editorial: Breaking the Discovery Impasse (part 1): A Case for Deep Learning. Combinatorial Chemistry and High Throughput Screening, 2018, 21, 3-4.	0.6	1
152	GOAPhAR: An Integrative Discovery Tool for Annotation, Pathway Analysis. Open Bioinformatics Journal, 2009, 3, 26-30.	1.0	1
153	Acetylcholinesterase Reprised: Molecular Modeling with the Whole Toolkit. , 2012, , 423-456.		1
154	Neuropharmacology in Flux: Molecular Modeling Tools for Understanding Protein Conformational Shifts in Alzheimerâ€™s Disease and Related Disorders. Neuromethods, 2018, , 573-611.	0.2	1
155	Occurrence of Antimicrobial Resistance Genes in the Oral Cavity of Cats with Chronic Gingivostomatitis. Animals, 2021, 11, 3589.	1.0	1
156	Defense against chemical warfare agents and toxic industrial chemicals. , 0, , .		0
157	Modular Synthesis of Cyclic Peptidomimetics Inspired by Î³-Turns.. ChemInform, 2005, 36, no.	0.1	0
158	Editorial [Hot Topic: Computational Approaches in Medicinal Chemistry: Surveys, Case Studies and Future Directions (Guest Editor: Gerald H. Lushington)]. Current Topics in Medicinal Chemistry, 2006, 6, 1-1.	1.0	0
159	Application of Kernel Functions for Accurate Similarity Search in Large Chemical Databases. , 2009, , .		0
160	Exploratory analysis of the BioAssay Network with implications to therapeutic discovery. , 2010, , .		0
161	Systematic data integration platform for functional glycomics. , 2010, , .		0
162	EVOL optimer - tool for gene expression analysis. , 2010, , .		0

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163	Similarity boosting for label noise tolerance in protein-chemical interaction prediction. , 2011, , .		0
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