Gerald Henry Lushington

List of Publications by Year
in descending order

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175	4,193	101384	161609
papers	citations	36 h-index	54 g-index

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

#	Article	IF	Citations
1	Occurrence of Antimicrobial Resistance Genes in the Oral Cavity of Cats with Chronic Gingivostomatitis. Animals, 2021, 11, 3589.	1.0	1
2	Structure-Guided Optimization of Dipeptidyl Inhibitors of Norovirus 3CL Protease. Journal of Medicinal Chemistry, 2020, 63, 11945-11963.	2.9	10
3	Perspective on the COVID-19 Coronavirus Outbreak. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 90-91.	0.6	2
4	Preface. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 3-3.	0.6	0
5	Chemistry, Screening, and the Democracy of Publishing. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 288-289.	0.6	2
6	Protein Glycation: An Old Villain is Shedding Secrets. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 362-369.	0.6	5
7	Meet Our Editor-in-Chief. Combinatorial Chemistry and High Throughput Screening, 2019, 22, 1-2.	0.6	0
8	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
9	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
10	Editorial: Breaking the Discovery Impasse (Part 2): Deep Learning New Tricks from Old Data. Combinatorial Chemistry and High Throughput Screening, 2018, 21, 234-235.	0.6	0
11	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
12	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
13	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
14	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
15	Chemical Informatics. , 2017, , 295-314.		0
16	Righting the Ship. , 2017, , 411-427.		0
17	Meet Our Editor. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 1-1.	0.6	4
18	Editorial: Great Science: Literature, Logic and a Bit of Modeling Glue. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 2-2.	0.6	0

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19	Editorial: Validate and Verify: Keys to Scientific Excellence. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 178-179.	0.6	0
20	Editorial: Beyond Pills and Needles: Delivering on New Promise. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 690-690.	0.6	0
21	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
22	Enantiospecific Synthesis and Cytotoxicity Evaluation of Oximidineâ€...II Analogues. ChemMedChem, 2016, 11, 1600-1616.	1.6	3
23	Oxadiazole-Based Cell Permeable Macrocyclic Transition State Inhibitors of Norovirus 3CL Protease. Journal of Medicinal Chemistry, 2016, 59, 1899-1913.	2.9	24
24	Biomedical research: a house of cards?. Future Medicinal Chemistry, 2016, 8, 1-5.	1.1	7
25	Editorial: Pits (and Plums?) in the Mire of Medical Talk Shows. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 440-441.	0.6	0
26	Editorial: In Memorium, Professor Lester Mitscher. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 832-833.	0.6	0
27	Comparative Modeling of Proteins. Methods in Molecular Biology, 2015, 1215, 309-330.	0.4	9
28	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
29	Editorial: Chemical Screening: Thinking Big with Big Data. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 483-484.	0.6	0
30	Editorial: Computational Toxicology: Screening, Chemistry, or Much More?. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 733-733.	0.6	1
31	Editorial: Mining for Pharmacophores in Phenotypic Screens. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 651-651.	0.6	1
32	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
33	Cloning and characterization of feline islet glucokinase. BMC Veterinary Research, 2014, 10, 130.	0.7	0
34	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
35	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
36	Potent inhibition of norovirus by dipeptidyl Î±-hydroxyphosphonate transition state mimics. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5941-5944.	1.0	25

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37	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
38	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
39	Solution-Phase Parallel Synthesis of a Multisubstituted Cyclic Imidate Library. ACS Combinatorial Science, 2013, 15, 247-254.	3.8	17
40	Chemical Informatics and the Drug Discovery Knowledge Pyramid. Combinatorial Chemistry and High Throughput Screening, 2013, 16, 764-776.	0.6	3
41	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
42	Synthesis of an Isoindoline-Annulated, Tricyclic Sultam Library via Microwave-Assisted, Continuous-Flow Organic Synthesis (MACOS). Synthesis, 2012, 44, 2547-2554.	1.2	24
43	Multi-target protein-chemical interaction prediction using task-regularized and boosted multi-task learning. , 2012, , .		1
44	Solution-Phase Synthesis of a Highly Substituted Furan Library. ACS Combinatorial Science, 2012, 14, 403-414.	3.8	33
45	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
46	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
47	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
48	Facile (Triazolyl)methylation of MACOS-derived Benzofused Sultams Utilizing ROMP-derived OTP Reagents. ACS Combinatorial Science, 2012, 14, 268-272.	3.8	20
49	Inhibitors of membranous adenylyl cyclases. Trends in Pharmacological Sciences, 2012, 33, 64-78.	4.0	90
50	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
51	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
52	Exploring chemical diversity via a modular reaction pairing strategy. Beilstein Journal of Organic Chemistry, 2012, 8, 1293-1302.	1.3	5
53	Differentiating between Models of Epothilone Binding to Microtubules Using Tubulin Mutagenesis, Cytotoxicity, and Molecular Modeling. ChemMedChem, 2012, 7, 1580-1586.	1.6	7
54	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

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55	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
56	Acetylcholinesterase Reprised: Molecular Modeling with the Whole Toolkit. , 2012, , 423-456.		1
57	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
58	Automated Synthesis of a 184-Member Library of Thiadiazepan-1,1-dioxide-4-ones. ACS Combinatorial Science, 2011, 13, 244-250.	3.8	19
59	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
60	Synthesis of Amino-Benzothiaoxazepine-1,1-dioxides Utilizing a Microwave-Assisted, S_NAr Protocol. ACS Combinatorial Science, 2011, 13, 653-658.	3.8	13
61	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
62	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
63	A filter-based feature selection approach for identifying potential biomarkers for lung cancer. Journal of Clinical Bioinformatics, 2011, 1, 11.	1.2	45
64	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
65	Design, synthesis, and evaluation of inhibitors of Norwalk virus 3C protease. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5315-5319.	1.0	46
66	Solution-Phase Parallel Synthesis of a Diverse Library of 1,2-Dihydroisoquinolines. ACS Combinatorial Science, 2011, 13, 265-271.	3.8	54
67	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
68	LipidomeDB Data Calculation Environment: Online Processing of Directâ€Infusion Mass Spectral Data for Lipid Profiles. Lipids, 2011, 46, 879-884.	0.7	49
69	The BioAssay network and its implications to future therapeutic discovery. BMC Bioinformatics, 2011, 12, S1.	1.2	15
70	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
71	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
72	Similarity boosting for label noise tolerance in protein-chemical interaction prediction. , 2011, , .		0

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73	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
74	GlycomicsDB - A Data Integration Platform for Glycans and their Strucutres. Open Medical Informatics Journal, 2011, 5, 9-17.	1.0	2
75	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
76	Application of kernel functions for accurate similarity search in large chemical databases. BMC Bioinformatics, 2010, 11, S8.	1.2	9
77	Exploratory analysis of the BioAssay Network with implications to therapeutic discovery. , 2010, , .		0
78	Crystal Structure of Histamine Dehydrogenase from Nocardioides simplex. Journal of Biological Chemistry, 2010, 285, 25782-25791.	1.6	16
79	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
80	Systematic data integration platform for functional glycomics. , 2010, , .		0
81	EVOL optimer - tool for gene expression analysis. , 2010, , .		0
82	S_NAr-Based, Facile Synthesis of a Library of Benzothiaoxazepine-1,1â€²-dioxides. ACS Combinatorial Science, 2010, 12, 850-854.	3.3	20
83	Reagent based DOS: A â€œClick, Click, Cyclizeâ€•strategy to probe chemical space. Organic and Biomolecular Chemistry, 2010, 8, 2198.	1.5	40
84	Uptake, Distribution and Diffusivity of Reactive Fluorophores in Cells: Implications toward Target Identification. Molecular Pharmaceutics, 2010, 7, 1301-1310.	2.3	49
85	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
86	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
87	GRAPH WAVELET ALIGNMENT KERNELS FOR DRUG VIRTUAL SCREENING. Journal of Bioinformatics and Computational Biology, 2009, 07, 473-497.	0.3	25
88	Key Residues Controlling Binding of Diverse Ligands to Human Cytochrome P450 2A Enzymes. Drug Metabolism and Disposition, 2009, 37, 1319-1327.	1.7	40
89	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
90	G-hash. , 2009, 360, 472-480.		27

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91	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
92	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
93	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
94	Notice of Violation of IEEE Publication Principles - Systematically Identifying Genes and Pathways in Multiple Cancer Types Using HGD & PSO-SVM. , 2009, , .		2
95	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
96	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
97	CGM: A biomedical text categorization approach using concept graph mining. , 2009, , .		5
98	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
99	Solution-Phase Parallel Synthesis of a Multi-substituted Benzo[b]thiophene Library. ACS Combinatorial Science, 2009, 11, 900-906.	3.3	55
100	Feature Selection in the Tensor Product Feature Space. , 2009, , 1004-1009.		10
101	Application of Kernel Functions for Accurate Similarity Search in Large Chemical Databases. , 2009, , .		0
102	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
103	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
104	GOAPhAR: An Integrative Discovery Tool for Annotation, Pathway Analysis. Open Bioinformatics Journal, 2009, 3, 26-30.	1.0	1
105	Differences in Paclitaxel and Docetaxel Interactions with Tubulin Detected by Mutagenesis of Yeast Tubulin. ChemMedChem, 2008, 3, 1844-1847.	1.6	15
106	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
107	The paclitaxel site in tubulin probed by siteâ€directed mutagenesis of Saccharomyces cerevisiae Î²â€tubulin. FEBS Letters, 2008, 582, 2467-2470.	1.3	12
108	Parallel Synthesis of a Multi-Substituted Benzo[b]furan Library. ACS Combinatorial Science, 2008, 10, 941-947.	3.3	59

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109	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
110	Comparative Modeling of Proteins. Methods in Molecular Biology, 2008, 443, 199-212.	0.4	5
111	Solution Phase Synthesis of a Diverse Library of Highly Substituted Isoxazoles. ACS Combinatorial Science, 2008, 10, 658-663.	3.3	67
112	GPM: A graph pattern matching kernel with diffusion for chemical compound classification. , 2008, 2008, 1-6.		25
113	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
114	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
115	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
116	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
117	FEATURE SELECTION IN VALIDATING MASS SPECTROMETRY DATABASE SEARCH RESULTS. Journal of Bioinformatics and Computational Biology, 2008, 06, 223-240.	0.3	10
118	Activation and Inhibition of Adenylyl Cyclase Isoforms by Forskolin Analogs. Journal of Pharmacology and Experimental Therapeutics, 2008, 325, 27-36.	1.3	81
119	Novel Algorithms for the Identification of Biologically Informative Chemical Diversity Metrics. Current Computer-Aided Drug Design, 2008, 4, 23-34.	0.8	3
120	Rat Cardiomyocytes Express a Classical Epithelial Beta-Defensin. American Journal of Animal and Veterinary Sciences, 2008, 3, 1-6.	0.2	8
121	GRAPH WAVELET ALIGNMENT KERNELS FOR DRUG VIRTUAL SCREENING. , 2008, , .		4
122	Whither Combine? New Opportunities for Receptor-Based QSAR. Current Medicinal Chemistry, 2007, 14, 1863-1877.	1.2	37
123	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
124	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
125	Structure of the Human Lung Cytochrome P450 2A13. Journal of Biological Chemistry, 2007, 282, 17306-17313.	1.6	90
126	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

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127	Encircled Proton. Journal of the American Chemical Society, 2007, 129, 8692-8693.	6.6	51
128	One-Step Synthesis of Oxazoline and Dihydrooxazine Libraries. ACS Combinatorial Science, 2007, 9, 473-476.	3.3	45
129	Solution-Phase Parallel Synthesis of a Library of Î”2-Pyrazolines. ACS Combinatorial Science, 2007, 9, 20-28.	3.3	24
130	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
131	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
132	Bioinformatics process management: information flow via a computational journal. Source Code for Biology and Medicine, 2007, 2, 9.	1.7	4
133	Stability and Electronic Properties of Nitrogen Nanoneedles and Nanotubes. Journal of Chemical Information and Modeling, 2006, 46, 1965-1971.	2.5	13
134	Monte Carlo simulations of CO2-expanded acetonitrile. Molecular Physics, 2006, 104, 2955-2960.	0.8	9
135	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
136	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
137	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
138	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
139	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
140	Acetylcholinesterase: Molecular Modeling with the Whole Toolkit. Current Topics in Medicinal Chemistry, 2006, 6, 57-73.	1.0	21
141	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
142	Support Vector Machines in HTS Data Mining: Type I MetAPs Inhibition Study. Journal of Biomolecular Screening, 2006, 11, 138-144.	2.6	13
143	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
144	Interactions of organophosphorus and related compounds with cholinesterases, a theoretical study. Chemico-Biological Interactions, 2005, 157-158, 321-325.	1.7	8

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145	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
146	Discover protein sequence signatures from protein-protein interaction data. BMC Bioinformatics, 2005, 6, 277.	1.2	20
147	Deamidation of model Î²-turn cyclic peptides in the solid state. Journal of Pharmaceutical Sciences, 2005, 94, 2616-2631.	1.6	10
148	Modular Synthesis of Cyclic Peptidomimetics Inspired by Î³-Turns.. ChemInform, 2005, 36, no.	0.1	0
149	Novel splice isoforms for NLGN3 and NLGN4 with possible implications in autism. Journal of Medical Genetics, 2005, 43, e21-e21.	1.5	148
150	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
151	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
152	Orientational Dynamics and Dye-DNA Interactions in a Dye-Labeled DNA Aptamer. Biophysical Journal, 2005, 88, 3455-3465.	0.2	94
153	Modular Synthesis of Cyclic Peptidomimetics Inspired by Î³-Turnsâ€. Organic Letters, 2005, 7, 1059-1062.	2.4	37
154	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
155	Organometallic Isocyanocyclopentadienides:Â A Combined Synthetic, Spectroscopic, Structural, Electrochemical, and Theoretical Investigation. Organometallics, 2004, 23, 2927-2938.	1.1	34
156	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
157	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
158	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
159	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
160	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
161	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
162	First Isocyanoazulene and Its Homoleptic Complexes. Journal of the American Chemical Society, 2003, 125, 4432-4433.	6.6	20

#	Article	IF	Citations
163	First Homoleptic Complexes of Isocyanoferrocene. Journal of the American Chemical Society, 2002, 124, 13668-13669.	6.6	31
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