List of Publications by Year in descending order

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205 papers	9,759 citations	26630 56 h-index	51608 86 g-index
214 all docs	214 docs citations	214 times ranked	6813 citing authors

#	Article	IF	Citations
1	Synthesis and study of the trypanocidal activity of catechol-containing 3-arylcoumarins, inclusion in Î²-cyclodextrin complexes and combination with benznidazole. Arabian Journal of Chemistry, 2022, 15, 103641.	4.9	1
2	Coumarin-Resveratrol-Inspired Hybrids as Monoamine Oxidase B Inhibitors: 3-Phenylcoumarin versusÂtrans-6-Styrylcoumarin. Molecules, 2022, 27, 928.	3.8	13
3	Design and synthesis of chromone-based monoamine oxidase B inhibitors with improved drug-like properties. European Journal of Medicinal Chemistry, 2022, 239, 114507.	5.5	6
4	7â€Amidocoumarins as Multitarget Agents against Neurodegenerative Diseases: Substitution Pattern Modulation. ChemMedChem, 2021, 16, 179-186.	3.2	13
5	Chemical and biological analysis of 4-acyloxy-3-nitrocoumarins as trypanocidal agents. Arabian Journal of Chemistry, 2021, 14, 102975.	4.9	3
6	4-Oxoquinolines and monoamine oxidase: When tautomerism matters. European Journal of Medicinal Chemistry, 2021, 213, 113183.	5.5	8
7	Combined 3D-QSAR and docking analysis for the design and synthesis of chalcones as potent and selective monoamine oxidase B inhibitors. Bioorganic Chemistry, 2021, 108, 104689.	4.1	26
8	Curcuminâ€“Coumarin Hybrid Analogues as Multitarget Agents in Neurodegenerative Disorders. Molecules, 2021, 26, 4550.	3.8	8
9	Study of a Selected Series of 3â€•and 4â€Arylcoumarins as Antifungal Agents against Dermatophytic Fungi: T. rubrum and T. mentagrophytes. ChemistrySelect, 2021, 6, 9981-9989.	1.5	0
10	3-Phenylcoumarins as a Privileged Scaffold in Medicinal Chemistry: The Landmarks of the Past Decade. Molecules, 2021, 26, 6755.	3.8	6
11	Structure-Based Optimization of Coumarin hA₃ Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2020, 63, 2577-2587.	6.4	14
12	Adenosine Receptor Ligands: Coumarinâ€“Chalcone Hybrids as Modulating Agents on the Activity of hARs. Molecules, 2020, 25, 4306.	3.8	8
13	3-Arylcoumarins as highly potent and selective monoamine oxidase B inhibitors: Which chemical features matter?. Bioorganic Chemistry, 2020, 101, 103964.	4.1	16
14	Discovery and optimization of 3-thiophenylcoumarins as novel agents against Parkinsonâ€™s disease: Synthesis, in vitro and in vivo studies. Bioorganic Chemistry, 2020, 101, 103986.	4.1	14
15	Looking for new xanthine oxidase inhibitors: 3-Phenylcoumarins versus 2-phenylbenzofurans. International Journal of Biological Macromolecules, 2020, 162, 774-780.	7.5	19
16	Coumarinâ€Rasagiline Hybrids as Potent and Selective hMAOâ€B Inhibitors, Antioxidants, and Neuroprotective Agents. ChemMedChem, 2020, 15, 532-538.	3.2	20
17	Antibacterial Activity and Molecular Docking Studies of a Selected Series of Hydroxy-3-arylcoumarins. Molecules, 2019, 24, 2815.	3.8	69
18	Design, Synthesis and Docking Calculations of Prenylated Chalcones as Selective Monoamine Oxidase B Inhibitors with Antioxidant Activity. ChemistrySelect, 2019, 4, 7698-7703.	1.5	19

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19	Quercetin and Related Chromenone Derivatives as Monoamine Oxidase Inhibitors: Targeting Neurological and Mental Disorders. Molecules, 2019, 24, 418.	3.8	63
20	Insights into the Discovery of Novel Neuroprotective Agents: A Comparative Study between Sulfanylcinnamic Acid Derivatives and Related Phenolic Analogues. Molecules, 2019, 24, 4405.	3.8	11
21	Novel Coumarinâ€Quinoline Hybrids: Design of Multitarget Compounds for Alzheimer's Disease. ChemistrySelect, 2019, 4, 551-558.	1.5	21
22	Tight-Binding Inhibition of Human Monoamine Oxidase B by Chromone Analogs: A Kinetic, Crystallographic, and Biological Analysis. Journal of Medicinal Chemistry, 2018, 61, 4203-4212.	6.4	58
23	PEGylated PLGA Nanoparticles As a Smart Carrier to Increase the Cellular Uptake of a Coumarin-Based Monoamine Oxidase B Inhibitor. ACS Applied Materials & Interfaces, 2018, 10, 39557-39569.	8.0	37
24	Multi-target-directed ligands for Alzheimer's disease: Discovery of chromone-based monoamine oxidase/cholinesterase inhibitors. European Journal of Medicinal Chemistry, 2018, 158, 781-800.	5.5	58
25	Coumarin derivatives as promising xanthine oxidase inhibitors. International Journal of Biological Macromolecules, 2018, 120, 1286-1293.	7.5	46
26	New insights into highly potent tyrosinase inhibitors based on 3-heteroarylcoumarins: Anti-melanogenesis and antioxidant activities, and computational molecular modeling studies. Bioorganic and Medicinal Chemistry, 2017, 25, 1687-1695.	3.0	53
27	Synthesis and structure-activity relationship study of novel 3-heteroarylcoumarins based on pyridazine scaffold as selective MAO-B inhibitors. European Journal of Medicinal Chemistry, 2017, 139, 1-11.	5.5	39
28	Coumarin versus Chromone Monoamine Oxidase B Inhibitors: Quo Vadis?. Journal of Medicinal Chemistry, 2017, 60, 7206-7212.	6.4	47
29	Structural elucidation of a series of 6â€methylâ€3â€carboxamidocoumarins. Magnetic Resonance in Chemistry, 2017, 55, 373-378.	1.9	2
30	Synthesis, antioxidant and antichagasic properties of a selected series of hydroxy-3-arylcoumarins. Bioorganic and Medicinal Chemistry, 2017, 25, 621-632.	3.0	34
31	Evaluation of Antioxidant and Antitrypanosomal Properties of a Selected Series of Synthetic 3â€Carboxamidocoumarins. ChemistrySelect, 2016, 1, 4957-4964.	1.5	3
32	Development of Bloodâ€“Brain Barrier Permeable Nitrocatechol-Based Catechol O-Methyltransferase Inhibitors with Reduced Potential for Hepatotoxicity. Journal of Medicinal Chemistry, 2016, 59, 7584-7597.	6.4	32
33	Computational Drug Target Screening through Protein Interaction Profiles. Scientific Reports, 2016, 6, 36969.	3.3	9
34	Discovery of New Chemical Entities for Old Targets: Insights on the Lead Optimization of Chromone-Based Monoamine Oxidase B (MAO-B) Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 5879-5893.	6.4	87
35	3â€Amidocoumarins as Potential Multifunctional Agents against Neurodegenerative Diseases. ChemMedChem, 2015, 10, 2071-2079.	3.2	24
36	Bioactive Coumarins from Marine Sources: Origin, Structural Features and Pharmacological Properties. Current Topics in Medicinal Chemistry, 2015, 15, 1755-1766.	2.1	22

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37	Study of Coumarin-Resveratrol Hybrids as Potent Antioxidant Compounds. Molecules, 2015, 20, 3290-3308.	3.8	37
38	Development of novel adenosine receptor ligands based on the 3-amidocoumarin scaffold. Bioorganic Chemistry, 2015, 61, 1-6.	4.1	9
39	Potential pharmacological uses of chalcones: a patent review (from June 2011 â€“ 2014). Expert Opinion on Therapeutic Patents, 2015, 25, 351-366.	5.0	125
40	Potent and selective MAO-B inhibitory activity: Amino- versus nitro-3-arylcoumarin derivatives. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 642-648.	2.2	28
41	Design, synthesis and antibacterial study of new potent and selective coumarinâ€“chalcone derivatives for the treatment of tenacibaculosis. Bioorganic and Medicinal Chemistry, 2015, 23, 7045-7052.	3.0	36
42	Insight into the Interactions between Novel Coumarin Derivatives and Human A₃ Adenosine Receptors. ChemMedChem, 2014, 9, 2245-2253.	3.2	13
43	Chromone: A Valid Scaffold in Medicinal Chemistry. Chemical Reviews, 2014, 114, 4960-4992.	47.7	576
44	Insight into the Functional and Structural Properties of 3â€Arylcoumarin as an Interesting Scaffold in Monoamine Oxidaseâ€...B Inhibition. ChemMedChem, 2014, 9, 1488-1500.	3.2	35
45	Monoamine Oxidase (MAO) Inhibitory Activity: 3â€Phenylcoumarins versus 4â€Hydroxyâ€3â€phenylcoumarins. ChemMedChem, 2014, 9, 1672-1676.	3.2	16
46	Similarity-based modeling in large-scale prediction of drug-drug interactions. Nature Protocols, 2014, 9, 2147-2163.	12.0	178
47	Synthesis, pharmacological study and docking calculations of new benzo[f]coumarin derivatives as dual inhibitors of enzymatic systems involved in neurodegenerative diseases. Future Medicinal Chemistry, 2014, 6, 371-383.	2.3	28
48	Synthesis and electrochemical study of new 3-(hydroxyphenyl)benzo[f]coumarins. Journal of Electroanalytical Chemistry, 2014, 726, 62-70.	3.8	6
49	State of the Art and Development of a Drug-Drug Interaction Large Scale Predictor Based on 3D Pharmacophoric Similarity. Current Drug Metabolism, 2014, 15, 490-501.	1.2	16
50	Synthesis and Electrochemical and Biological Studies of Novel Coumarinâ€“Chalcone Hybrid Compounds. Journal of Medicinal Chemistry, 2013, 56, 6136-6145.	6.4	82
51	Remarkable antioxidant properties of a series of hydroxy-3-arylcoumarins. Bioorganic and Medicinal Chemistry, 2013, 21, 3900-3906.	3.0	55
52	Classifier Ensemble Based on Feature Selection and Diversity Measures for Predicting the Affinity of A2BAdenosine Receptor Antagonists. Journal of Chemical Information and Modeling, 2013, 53, 3140-3155.	5.4	12
53	Synthesis and adenosine receptors binding affinities of a series of 3-arylcoumarins. Journal of Pharmacy and Pharmacology, 2013, 65, 1590-1597.	2.4	16
54	Comparative study of the 3-phenylcoumarin scaffold: Synthesis, X-ray structural analysis and semiempirical calculations of a selected series of compounds. Journal of Molecular Structure, 2013, 1050, 185-191.	3.6	2

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55	Synthesis and NMR studies of novel chromoneâ€2â€carboxamide derivatives. Magnetic Resonance in Chemistry, 2013, 51, 251-254.	1.9	7
56	New hydroxylated 3-arylcoumarins, synthesis and electrochemical study. Journal of Electroanalytical Chemistry, 2013, 689, 243-251.	3.8	9
57	MAO Inhibitory Activity of 2â€Arylbenzofurans versus 3â€Arylcoumarins: Synthesis, inâ€...vitro Study, and Docking Calculations. ChemMedChem, 2013, 8, 956-966.	3.2	32
58	Synthesis and Structure-Activity Relationships of Novel Amino/Nitro Substituted 3-Arylcoumarins as Antibacterial Agents. Molecules, 2013, 18, 1394-1404.	3.8	59
59	Novel (coumarin-3-yl)carbamates as selective MAO-B inhibitors: Synthesis, inÂvitro and inÂvivo assays, theoretical evaluation of ADMEÂproperties and docking study. European Journal of Medicinal Chemistry, 2013, 63, 151-161.	5.5	50
60	Chalcone-based derivatives as new scaffolds for hA3 adenosine receptor antagonists. Journal of Pharmacy and Pharmacology, 2013, 65, 697-703.	2.4	44
61	Synthesis of coumarinâ€“chalcone hybrids and evaluation of their antioxidant and trypanocidal properties. MedChemComm, 2013, 4, 993.	3.4	66
62	Synthesis, NMR characterization, X-ray structural analysis and theoretical calculations of amide and ester derivatives of the coumarin scaffold. Journal of Molecular Structure, 2013, 1041, 144-150.	3.6	5
63	Synthesis and evaluation of antioxidant and trypanocidal properties of a selected series of coumarin derivatives. Future Medicinal Chemistry, 2013, 5, 1911-1922.	2.3	26
64	3-(4-Methoxybenzoyl)-6-nitrocoumarin. Acta Crystallographica Section E: Structure Reports Online, 2013, 69, o345-o345.	0.2	1
65	Detection of Drug-Drug Interactions by Modeling Interaction Profile Fingerprints. PLoS ONE, 2013, 8, e58321.	2.5	96
66	Focusing on New Monoamine Oxidase Inhibitors: Differently Substituted Coumarins As An Interesting Scaffold. Current Topics in Medicinal Chemistry, 2012, 12, 2210-2239.	2.1	68
67	Monoamine Oxidase Inhibitors: Ten Years of Docking Studies. Current Topics in Medicinal Chemistry, 2012, 12, 2145-2162.	2.1	31
68	Drugâ€”drug interaction through molecular structure similarity analysis. Journal of the American Medical Informatics Association: JAMIA, 2012, 19, 1066-1074.	4.4	185
69	3-Phenylcoumarin. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o2645-o2645.	0.2	7
70	N-(2-Oxo-2H-chromen-3-yl)cyclohexanecarboxamide. Acta Crystallographica Section E: Structure Reports Online, 2012, 68, o3447-o3448.	0.2	0
71	Looking for New Targets: Simple Coumarins as Antibacterial Agents. Medicinal Chemistry, 2012, 8, 1140-1145.	1.5	5
72	In search for new chemical entities as adenosine receptor ligands: Development of agents based on benzo-Î³-pyrone skeleton. European Journal of Medicinal Chemistry, 2012, 54, 914-918.	5.5	27

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73	Improved Synthesis of 3-(Aminoaryl)coumarins. Organic Preparations and Procedures International, 2012, 44, 522-526.	1.3	7
74	Antitrypanosomal and antioxidant properties of 4-hydroxycoumarins derivatives. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5569-5573.	2.2	48
75	Targeting adenosine receptors with coumarins: synthesis and binding activities of amide and carbamate derivatives. Journal of Pharmacy and Pharmacology, 2012, 65, 30-34.	2.4	13
76	Synthesis and cytotoxic activity of non-naturally substituted 4-oxycoumarin derivatives. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5791-5794.	2.2	26
77	Looking for New Targets: Simple Coumarins as Antibacterial Agents. Medicinal Chemistry, 2012, 8, 1140-1145.	1.5	61
78	Enhancing Adverse Drug Event Detection in Electronic Health Records Using Molecular Structure Similarity: Application to Pancreatitis. PLoS ONE, 2012, 7, e41471.	2.5	25
79	3-Substituted coumarins as dual inhibitors of AChE and MAO for the treatment of Alzheimer's disease. MedChemComm, 2012, 3, 213-218.	3.4	96
80	8â€Substituted 3â€Arylcoumarins as Potent and Selective MAOâ€B Inhibitors: Synthesis, Pharmacological Evaluation, and Docking Studies. ChemMedChem, 2012, 7, 464-470.	3.2	57
81	Discovery of novel A3 adenosine receptor ligands based on chromone scaffold. Biochemical Pharmacology, 2012, 84, 21-29.	4.4	46
82	A novel tetrahydrobenzoangelicin with dark and photo biological activity. Bioorganic and Medicinal Chemistry, 2012, 20, 3603-3608.	3.0	8
83	Hydroxycoumarins as selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 258-261.	2.2	53
84	Tyrosine-like condensed derivatives as tyrosinase inhibitors. Journal of Pharmacy and Pharmacology, 2012, 64, 742-746.	2.4	16
85	Chromone, a Privileged Scaffold for the Development of Monoamine Oxidase Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 5165-5173.	6.4	140
86	Synthesis and Study of a Series of 3-Arylcoumarins as Potent and Selective Monoamine Oxidase B Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 7127-7137.	6.4	147
87	Rational design of new agrochemical fungicides using substructural descriptors. Pest Management Science, 2011, 67, 438-445.	3.4	33
88	Towards the Discovery of a Novel Class of Monoamine Oxidase Inhibitors: Structureâ€“Propertyâ€“Activity and Docking Studies on Chromone Amides. ChemMedChem, 2011, 6, 628-632.	3.2	34
89	Chromone 3-phenylcarboxamides as potent and selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 707-709.	2.2	76
90	New halogenated phenylcoumarins as tyrosinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 3342-3345.	2.2	63

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91	MAO inhibitory activity modulation: 3-Phenylcoumarins versus 3-benzoylcoumarins. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 4224-4227.	2.2	59
92	Synthesis, human monoamine oxidase inhibitory activity and molecular docking studies of 3-heteroarylcoumarin derivatives. European Journal of Medicinal Chemistry, 2011, 46, 1147-1152.	5.5	65
93	Using the TOPS-MODE approach to fit multi-target QSAR models for tyrosine kinases inhibitors. European Journal of Medicinal Chemistry, 2011, 46, 2185-2192.	5.5	62
94	Synthesis of 3-arylcoumarins via Suzuki-cross-coupling reactions of 3-chlorocoumarin. Tetrahedron Letters, 2011, 52, 1225-1227.	1.4	45
95	Designing novel antitrypanosomal agents from a mixed graphâ€theoretical substructural approach. Journal of Computational Chemistry, 2010, 31, 882-894.	3.3	27
96	Structural Contributions of Substrates to their Binding to P-Glycoprotein. A TOPSMODE Approach. Current Pharmaceutical Design, 2010, 16, 2676-2709.	1.9	41
97	Pyridazinopsoralens of wide chemotherapeutic interest. Bioorganic and Medicinal Chemistry, 2010, 18, 5708-5714.	3.0	3
98	Chromone-2- and -3-carboxylic acids inhibit differently monoamine oxidases A and B. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2709-2712.	2.2	47
99	New halogenated 3-phenylcoumarins as potent and selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5157-5160.	2.2	87
100	Regioselective Synthesis of Bromo-Substituted 3-Arylcoumarins. Synthesis, 2010, 2010, 2763-2766.	2.3	10
101	Protein Graphs in Cancer Prediction. , 2010, , 125-140.		1
102	Computational chemistry study of 3Dâ€structureâ€function relationships for enzymes based on Markov models for protein electrostatic, HINT, and van der Waals potentials. Journal of Computational Chemistry, 2009, 30, 1510-1520.	3.3	52
103	Multi-target QPDR classification model for human breast and colon cancer-related proteins using star graph topological indices. Journal of Theoretical Biology, 2009, 257, 303-311.	1.7	72
104	Multi-target spectral moments for QSAR and Complex Networks study of antibacterial drugs. European Journal of Medicinal Chemistry, 2009, 44, 4516-4521.	5.5	66
105	Design of novel antituberculosis compounds using graph-theoretical and substructural approaches. Molecular Diversity, 2009, 13, 445-458.	3.9	48
106	Alignment-free prediction of mycobacterial DNA promoters based on pseudo-folding lattice network or star-graph topological indices. Journal of Theoretical Biology, 2009, 256, 458-466.	1.7	36
107	A network-QSAR model for prediction of genetic-component biomarkers in human colorectal cancer. Journal of Theoretical Biology, 2009, 261, 449-458.	1.7	67
108	QSAR and complex network study of the chiral HMGR inhibitor structural diversity. Bioorganic and Medicinal Chemistry, 2009, 17, 165-175.	3.0	24

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109	Unified QSAR approach to antimicrobials. 4. Multi-target QSAR modeling and comparative multi-distance study of the giant components of antiviral drugâ€“drug complex networks. Bioorganic and Medicinal Chemistry, 2009, 17, 569-575.	3.0	106
110	A new psoralen derivative with enlarged antiproliferative properties. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 2874-2876.	2.2	14
111	A new series of 3-phenylcoumarins as potent and selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3268-3270.	2.2	124
112	Synthesis and evaluation of 6-methyl-3-phenylcoumarins as potent and selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 5053-5055.	2.2	104
113	Multi-target spectral moment: QSAR for antiviral drugs vs. different viral species. Analytica Chimica Acta, 2009, 651, 159-164.	5.4	32
114	Alignment-Free Prediction of a Drugâ^'Target Complex Network Based on Parameters of Drug Connectivity and Protein Sequence of Receptors. Molecular Pharmaceutics, 2009, 6, 825-835.	4.6	83
115	Alignment-Free Prediction of Polygalacturonases with Pseudofolding Topological Indices: Experimental Isolation from Coffea arabica and Prediction of a New Sequence. Journal of Proteome Research, 2009, 8, 2122-2128.	3.7	65
116	Prediction of Enzyme Classes from 3D Structure: A General Model and Examples of Experimental-Theoretic Scoring of Peptide Mass Fingerprints of Leishmania Proteins. Journal of Proteome Research, 2009, 8, 4372-4382.	3.7	81
117	Proteomics, networks and connectivity indices. Proteomics, 2008, 8, 750-778.	2.2	207
118	A Minireview of Available Skin Sensitization (Q)SARs/Expert Systems. QSAR and Combinatorial Science, 2008, 27, 60-76.	1.4	44
119	Synthesis and complete assignment of the ¹H and ¹³C NMR signals of some oxopyrancoumarin and oxofuropyrancoumarin derivatives. Magnetic Resonance in Chemistry, 2008, 46, 701-705.	1.9	2
120	QSAR model for alignmentâ€free prediction of human breast cancer biomarkers based on electrostatic potentials of protein pseudofolding HPâ€lattice networks. Journal of Computational Chemistry, 2008, 29, 2613-2622.	3.3	48
121	Stochastic molecular descriptors for polymers. 4. Study of complex mixtures with topological indices of mass spectra spiral and star networks: The blood proteome case. Polymer, 2008, 49, 5575-5587.	3.8	27
122	Quantitative Proteomeâ€“Property Relationships (QPPRs). Part 1: Finding biomarkers of organic drugs with mean Markov connectivity indices of spiral networks of blood mass spectra. Bioorganic and Medicinal Chemistry, 2008, 16, 9684-9693.	3.0	18
123	Multi-target QSPR assemble of a Complex Network for the distribution of chemicals to biphasic systems and biological tissues. Chemometrics and Intelligent Laboratory Systems, 2008, 94, 160-165.	3.5	13
124	Coumarin as Attractive Casein Kinase 2 (CK2) Inhibitor Scaffold: An Integrate Approach To Elucidate the Putative Binding Motif and Explain Structureâ€“Activity Relationships. Journal of Medicinal Chemistry, 2008, 51, 752-759.	6.4	123
125	Quantitative Structureâ^'Activity Relationship and Complex Network Approach to Monoamine Oxidase A and B Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 6740-6751.	6.4	109
126	Using spectral moments of spiral networks based on PSA/mass spectra outcomes to derive quantitative proteomeâ€“disease relationships (QPDRs) and predicting prostate cancer. Biochemical and Biophysical Research Communications, 2008, 372, 320-325.	2.1	34

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127	Medicinal Chemistry and Bioinformatics - Current Trends in Drugs Discovery with Networks Topological Indices. Current Topics in Medicinal Chemistry, 2007, 7, 1015-1029.	2.1	271
128	A Model for the Recognition of Protein Kinases Based on the Entropy of 3D van der Waals Interactions. Journal of Proteome Research, 2007, 6, 904-908.	3.7	78
129	2D-RNA-coupling numbers: A new computational chemistry approach to link secondary structure topology with biological function. Journal of Computational Chemistry, 2007, 28, 1049-1056.	3.3	58
130	Computational chemistry comparison of stable/nonstable protein mutants classification models based on 3D and topological indices. Journal of Computational Chemistry, 2007, 28, 1990-1995.	3.3	61
131	Computational chemistry development of a unified free energy Markov model for the distribution of 1300 chemicals to 38 different environmental or biological systems. Journal of Computational Chemistry, 2007, 28, 1909-1923.	3.3	79
132	Assignment of the1H and13C NMR signals of some hydroxyphenylcoumarins. Magnetic Resonance in Chemistry, 2007, 45, 99-101.	1.9	3
133	QSAR study of anticoccidial activity for diverse chemical compounds: Prediction and experimental assay of trans-2-(2-nitrovinyl)furan. Bioorganic and Medicinal Chemistry, 2007, 15, 962-968.	3.0	24
134	Unified QSAR approach to antimicrobials. Part 2: Predicting activity against more than 90 different species in order to halt antibacterial resistance. Bioorganic and Medicinal Chemistry, 2007, 15, 897-902.	3.0	70
135	On the applicability of QSAR for recognition of miRNA bioorganic structures at early stages of organism and cell development: Embryo and stem cells. Bioorganic and Medicinal Chemistry, 2007, 15, 2544-2550.	3.0	25
136	ANN-QSAR model for selection of anticancer leads from structurally heterogeneous series of compounds. European Journal of Medicinal Chemistry, 2007, 42, 580-585.	5.5	67
137	Chemometrics for QSAR with low sequence homology: Mycobacterial promoter sequences recognition with 2D-RNA entropies. Chemometrics and Intelligent Laboratory Systems, 2007, 85, 20-26.	3.5	30
138	Quantitative Structure Vasodilatory Activity Relationship â€“ Synthesis and â€œIn Silicoâ€•and â€œIn Vitroâ€• Evaluation of Resveratrol-Coumarin Hybrids. QSAR and Combinatorial Science, 2007, 26, 317-332.	1.4	11
139	Probabilistic Neural Network Model for the In Silico Evaluation of Anti-HIV Activity and Mechanism of Action. Journal of Medicinal Chemistry, 2006, 49, 1118-1124.	6.4	80
140	An Integrated in Silico Analysis of Drug-Binding to Human Serum Albumin. Journal of Chemical Information and Modeling, 2006, 46, 2709-2724.	5.4	65
141	Effect of Protein Backbone Folding on the Stability of Proteinâ˜Ligand Complexes. Journal of Proteome Research, 2006, 5, 105-111.	3.7	19
142	New Furan Side Tetracyclic Allopsoralen Derivatives:Â Synthesis and Photobiological Evaluation. Journal of Medicinal Chemistry, 2006, 49, 4317-4326.	6.4	17
143	Novel 2D maps and coupling numbers for protein sequences. The first QSAR study of polygalacturonases; isolation and prediction of a novel sequence fromPsidium guajavaL.. FEBS Letters, 2006, 580, 723-730.	2.8	94
144	A QSAR Model for in Silico Screening of MAO-A Inhibitors. Prediction, Synthesis, and Biological Assay of Novel Coumarinsâ€. Journal of Medicinal Chemistry, 2006, 49, 1149-1156.	6.4	140

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145	Synthesis and Anti-HIV Activity of Novel Cyclopentenyl Nucleoside Analogues of 8-Azapurine. Chemical and Pharmaceutical Bulletin, 2006, 54, 1418-1420.	1.3	9
146	Unify QSAR approach to antimicrobials. Part 1: Predicting antifungal activity against different species. Bioorganic and Medicinal Chemistry, 2006, 14, 5973-5980.	3.0	69
147	Design, synthesis, and vasorelaxant and platelet antiaggregatory activities of coumarinâ€“resveratrol hybrids. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 257-261.	2.2	140
148	Stochastic entropy QSAR for the in silico discovery of anticancer compounds: Prediction, synthesis, and in vitro assay of new purine carbanucleosides. Bioorganic and Medicinal Chemistry, 2006, 14, 1095-1107.	3.0	25
149	Regioselective synthesis of O2- and O6-cyclopyrimidine nucleoside analogues. Tetrahedron, 2006, 62, 9949-9952.	1.9	8
150	QSAR study for mycobacterial promoters with low sequence homology. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 547-553.	2.2	35
151	Simple Stochastic Fingerprints Towards Mathematical Modeling in Biology and Medicine 2. Unifying Markov Model for Drugs Side Effects. Bulletin of Mathematical Biology, 2006, 68, 1527-1554.	1.9	9
152	Assignment of the1H and13C NMR signals of some benzofurocoumarins. Magnetic Resonance in Chemistry, 2006, 44, 644-647.	1.9	3
153	Stochastic molecular descriptors for polymers. 2. Spherical truncation of electrostatic interactions on entropy based polymers 3D-QSAR. Polymer, 2005, 46, 2791-2798.	3.8	31
154	Stochastic molecular descriptors for polymers. 3. Markov electrostatic moments as polymer 2D-folding descriptors: RNAâ€“QSAR for mycobacterial promoters. Polymer, 2005, 46, 6461-6473.	3.8	21
155	Predicting stability of Arc repressor mutants with protein stochastic moments. Bioorganic and Medicinal Chemistry, 2005, 13, 323-331.	3.0	52
156	Design, synthesis and photobiological properties of 3,4-cyclopentenepsoralens. Bioorganic and Medicinal Chemistry, 2005, 13, 809-817.	3.0	28
157	Predicting multiple drugs side effects with a general drug-target interaction thermodynamic Markov model. Bioorganic and Medicinal Chemistry, 2005, 13, 1119-1129.	3.0	47
158	3D QSAR Markov model for drug-induced eosinophiliaâ€”theoretical prediction and preliminary experimental assay of the antimicrobial drug G1. Bioorganic and Medicinal Chemistry, 2005, 13, 1523-1530.	3.0	28
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