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	Chromone: A Valid Scaffold in Medicinal Chemistry. Chemical Reviews, 2014, 114, 4960-4992.	47.7	576
2	Recent Advances on the Role of Topological Indices in Drug Discovery Research. Current Medicinal Chemistry, 2001, 8, 1573-1588.	2.4	279
3	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
4	Proteomics, networks and connectivity indices. Proteomics, 2008, 8, 750-778.	2.2	207
5	Drugâ€”drug interaction through molecular structure similarity analysis. Journal of the American Medical Informatics Association: JAMIA, 2012, 19, 1066-1074.	4.4	185
6	Similarity-based modeling in large-scale prediction of drug-drug interactions. Nature Protocols, 2014, 9, 2147-2163.	12.0	178
7	A Novel Approach for the Virtual Screening and Rational Design of Anticancer Compounds. Journal of Medicinal Chemistry, 2000, 43, 1975-1985.	6.4	176
8	Effects ofcis-resveratrol on inflammatory murine macrophages: antioxidant activity and down-regulation of inflammatory genes. Journal of Leukocyte Biology, 2004, 75, 1156-1165.	3.3	168
9	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
10	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
11	Design, synthesis, and vasorelaxant and platelet antiaggregatory activities of coumarinâ€“resveratrol hybrids. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 257-261.	2.2	140
12	Chromone, a Privileged Scaffold for the Development of Monoamine Oxidase Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 5165-5173.	6.4	140
13	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
14	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
15	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
16	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
17	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
18	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

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19	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
20	Detection of Drug-Drug Interactions by Modeling Interaction Profile Fingerprints. PLoS ONE, 2013, 8, e58321.	2.5	96
21	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
22	3D-MEDNEs:â€‰ An Alternative â€œIn Silicoâ€•Technique for Chemical Research in Toxicology. 1. Prediction of Chemically Induced Agranulocytosis. Chemical Research in Toxicology, 2003, 16, 1318-1327.	3.3	88
23	Markovian chemicals "in silico" design (MARCH-INSIDE), a promising approach for computer-aided molecular design I: discovery of anticancer compounds. Journal of Molecular Modeling, 2003, 9, 395-407.	1.8	87
24	New halogenated 3-phenylcoumarins as potent and selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5157-5160.	2.2	87
25	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
26	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
27	Designing Antibacterial Compounds through a Topological Substructural Approach. Journal of Chemical Information and Computer Sciences, 2004, 44, 515-521.	2.8	82
28	Synthesis and Electrochemical and Biological Studies of Novel Coumarinâ€“Chalcone Hybrid Compounds. Journal of Medicinal Chemistry, 2013, 56, 6136-6145.	6.4	82
29	Stochastic-based descriptors studying peptides biological properties: modeling the bitter tasting threshold of dipeptides. Bioorganic and Medicinal Chemistry, 2004, 12, 4815-4822.	3.0	81
30	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
31	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
32	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
33	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
34	Synthesis and Vasorelaxant Activity of New Coumarin and Furocoumarin Derivatives. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 783-786.	2.2	77
35	Coumarins â€” An Important Class of Phytochemicals. , 0, , .		77
36	Chromone 3-phenylcarboxamides as potent and selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 707-709.	2.2	76

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37	Markovian Backbone Negentropies: Molecular descriptors for protein research. I. Predicting protein stability in Arc repressor mutants. Proteins: Structure, Function and Bioinformatics, 2004, 56, 715-723.	2.6	74
38	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
39	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
40	Unify QSAR approach to antimicrobials. Part 1: Predicting antifungal activity against different species. Bioorganic and Medicinal Chemistry, 2006, 14, 5973-5980.	3.0	69
41	Antibacterial Activity and Molecular Docking Studies of a Selected Series of Hydroxy-3-arylcoumarins. Molecules, 2019, 24, 2815.	3.8	69
42	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
43	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
44	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
45	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
46	Synthesis of coumarinâ€“chalcone hybrids and evaluation of their antioxidant and trypanocidal properties. MedChemComm, 2013, 4, 993.	3.4	66
47	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
48	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
49	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
50	New halogenated phenylcoumarins as tyrosinase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 3342-3345.	2.2	63
51	Quercetin and Related Chromenone Derivatives as Monoamine Oxidase Inhibitors: Targeting Neurological and Mental Disorders. Molecules, 2019, 24, 418.	3.8	63
52	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
53	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
54	Looking for New Targets: Simple Coumarins as Antibacterial Agents. Medicinal Chemistry, 2012, 8, 1140-1145.	1.5	61

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55	In Silico Studies toward the Discovery of New Anti-HIV Nucleoside Compounds with the Use of TOPS-MODE and 2D/3D Connectivity Indices. 1. Pyrimidyl Derivatives. Journal of Chemical Information and Computer Sciences, 2002, 42, 1194-1203.	2.8	60
56	Markov entropy backbone electrostatic descriptors for predicting proteins biological activity. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 4691-4695.	2.2	59
57	MAO inhibitory activity modulation: 3-Phenylcoumarins versus 3-benzoylcoumarins. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 4224-4227.	2.2	59
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	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
60	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
61	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
62	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
63	Remarkable antioxidant properties of a series of hydroxy-3-arylcoumarins. Bioorganic and Medicinal Chemistry, 2013, 21, 3900-3906.	3.0	55
64	Symmetry considerations in Markovian chemicals â€˜in silicoâ€™ design (MARCH-INSIDE) I: central chirality codification, classification of ACE inhibitors and prediction of Ï*f*-receptor antagonist activities. Computational Biology and Chemistry, 2003, 27, 217-227.	2.3	54
65	New Tetracyclic Analogues of Photochemotherapeutic Drugs 5-MOP and 8-MOP:Â Synthesis, DNA Interaction, and Antiproliferative Activity. Journal of Medicinal Chemistry, 1999, 42, 4405-4413.	6.4	53
66	Markovian chemicals â€œin silicoâ€•design (MARCH-INSIDE), a promising approach for computer-aided molecular design III: 2.5D indices for the discovery of antibacterials. Journal of Molecular Modeling, 2005, 11, 116-123.	1.8	53
67	Hydroxycoumarins as selective MAO-B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 258-261.	2.2	53
68	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
69	Predicting stability of Arc repressor mutants with protein stochastic moments. Bioorganic and Medicinal Chemistry, 2005, 13, 323-331.	3.0	52
70	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
71	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
72	Recognition of stable protein mutants with 3D stochastic average electrostatic potentials. FEBS Letters, 2005, 579, 4297-4301.	2.8	48

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73	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
74	Design of novel antituberculosis compounds using graph-theoretical and substructural approaches. Molecular Diversity, 2009, 13, 445-458.	3.9	48
75	Antitrypanosomal and antioxidant properties of 4-hydroxycoumarins derivatives. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5569-5573.	2.2	48
76	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
77	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
78	Coumarin versus Chromone Monoamine Oxidase B Inhibitors: Quo Vadis?. Journal of Medicinal Chemistry, 2017, 60, 7206-7212.	6.4	47
79	Discovery of novel A3 adenosine receptor ligands based on chromone scaffold. Biochemical Pharmacology, 2012, 84, 21-29.	4.4	46
80	Coumarin derivatives as promising xanthine oxidase inhibitors. International Journal of Biological Macromolecules, 2018, 120, 1286-1293.	7.5	46
81	Unified Markov thermodynamics based on stochastic forms to classify drugs considering molecular structure, partition system, and biological species:. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 551-557.	2.2	45
82	Synthesis of 3-arylcoumarins via Suzuki-cross-coupling reactions of 3-chlorocoumarin. Tetrahedron Letters, 2011, 52, 1225-1227.	1.4	45
83	A Minireview of Available Skin Sensitization (Q)SARs/Expert Systems. QSAR and Combinatorial Science, 2008, 27, 60-76.	1.4	44
84	Chalcone-based derivatives as new scaffolds for hA3 adenosine receptor antagonists. Journal of Pharmacy and Pharmacology, 2013, 65, 697-703.	2.4	44
85	Peptidyl Anthraquinones as Potential Antineoplastic Drugs:â€‰ Synthesis, DNA Binding, Redox Cycling, and Biological Activity. Journal of Medicinal Chemistry, 1996, 39, 3114-3122.	6.4	41
86	Structural Contributions of Substrates to their Binding to P-Glycoprotein. A TOPSMODE Approach. Current Pharmaceutical Design, 2010, 16, 2676-2709.	1.9	41
87	AM1 theoretical study, synthesis and biological evaluation of some benzofuran analogues of anti-inflammatory arylalkanoic acids. European Journal of Pharmaceutical Sciences, 1999, 7, 161-166.	4.0	40
88	Stochastic molecular descriptors for polymers. 1. Modelling the properties of icosahedral viruses with 3D-Markovian negentropies. Polymer, 2004, 45, 3845-3853.	3.8	40
89	QSAR for anti-RNA-virus activity, synthesis, and assay of anti-RSV carbonucleosides given a unified representation of spectral moments, quadratic, and topologic indices. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1651-1657.	2.2	39
90	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

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91	Proteins Markovian 3D-QSAR with spherically-truncated average electrostatic potentials. Bioorganic and Medicinal Chemistry, 2005, 13, 3641-3647.	3.0	38
92	In Silico Studies toward the Discovery of New Anti-HIV Nucleoside Compounds through the Use of TOPS-MODE and 2D/3D Connectivity Indices. 2. Purine Derivatives. Journal of Chemical Information and Modeling, 2005, 45, 502-514.	5.4	38
93	Study of Coumarin-Resveratrol Hybrids as Potent Antioxidant Compounds. Molecules, 2015, 20, 3290-3308.	3.8	37
94	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
95	4â€˜-Methyl Derivatives of 5-MOP and 5-MOA:Â Synthesis, Photoreactivity, and Photobiological Activity. Journal of Medicinal Chemistry, 1996, 39, 4489-4496.	6.4	36
96	Proteins QSAR with Markov average electrostatic potentials. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5088-5094.	2.2	36
97	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
98	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
99	QSAR study for mycobacterial promoters with low sequence homology. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 547-553.	2.2	35
100	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
101	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
102	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
103	Synthesis, antioxidant and antichagasic properties of a selected series of hydroxy-3-arylcoumarins. Bioorganic and Medicinal Chemistry, 2017, 25, 621-632.	3.0	34
104	Rational design of new agrochemical fungicides using substructural descriptors. Pest Management Science, 2011, 67, 438-445.	3.4	33
105	2D RNA-QSAR: assigning ACC oxidase family membership with stochastic molecular descriptors; isolation and prediction of a sequence from Psidium guajava L. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 2932-2937.	2.2	32
106	Multi-target spectral moment: QSAR for antiviral drugs vs. different viral species. Analytica Chimica Acta, 2009, 651, 159-164.	5.4	32
107	MAO Inhibitory Activity of 2â€Arylbenzofurans versus 3â€Arylcoumarins: Synthesis, inâ€…vitro Study, and Docking Calculations. ChemMedChem, 2013, 8, 956-966.	3.2	32
108	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

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109	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
110	A furan ring expansion approach to the synthesis of novel pyridazino-psoralen derivatives. Tetrahedron, 2005, 61, 4805-4810.	1.9	31
111	Monoamine Oxidase Inhibitors: Ten Years of Docking Studies. Current Topics in Medicinal Chemistry, 2012, 12, 2145-2162.	2.1	31
112	Biopolymer stochastic moments. I. Modeling human rhinovirus cellular recognition with protein surface electrostatic moments. Biopolymers, 2005, 77, 296-303.	2.4	30
113	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
114	Design, synthesis and photobiological properties of 3,4-cyclopentenepsoralens. Bioorganic and Medicinal Chemistry, 2005, 13, 809-817.	3.0	28
115	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
116	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
117	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
118	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
119	Designing novel antitrypanosomal agents from a mixed graphâ€theoretical substructural approach. Journal of Computational Chemistry, 2010, 31, 882-894.	3.3	27
120	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
121	A new benzoangelicin with strong photobiological activity. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 135-137.	2.2	26
122	Synthesis and cytotoxic activity of non-naturally substituted 4-oxycoumarin derivatives. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 5791-5794.	2.2	26
123	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
124	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
125	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
126	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

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127	Enhancing Adverse Drug Event Detection in Electronic Health Records Using Molecular Structure Similarity: Application to Pancreatitis. PLoS ONE, 2012, 7, e41471.	2.5	25
128	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
129	QSAR and complex network study of the chiral HMGR inhibitor structural diversity. Bioorganic and Medicinal Chemistry, 2009, 17, 165-175.	3.0	24
130	3â€Amidocoumarins as Potential Multifunctional Agents against Neurodegenerative Diseases. ChemMedChem, 2015, 10, 2071-2079.	3.2	24
131	Bioactive Coumarins from Marine Sources: Origin, Structural Features and Pharmacological Properties. Current Topics in Medicinal Chemistry, 2015, 15, 1755-1766.	2.1	22
132	Novel Pyrone Side Tetracyclic Psoralen Derivatives:â€‰ Synthesis and Photobiological Evaluation. Journal of Medicinal Chemistry, 2003, 46, 3800-3810.	6.4	21
133	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
134	Novel Coumarinâ€Quinoline Hybrids: Design of Multitarget Compounds for Alzheimer's Disease. ChemistrySelect, 2019, 4, 551-558.	1.5	21
135	Inverse electron demand dielsâ€alder reactions of psoralens. Synthesis and mass spectra of novel pyridazinocoumarins. Journal of Heterocyclic Chemistry, 2000, 37, 907-910.	2.6	20
136	Coumarinâ€Rasagiline Hybrids as Potent and Selective hMAOâ€B Inhibitors, Antioxidants, and Neuroprotective Agents. ChemMedChem, 2020, 15, 532-538.	3.2	20
137	Effect of Protein Backbone Folding on the Stability of Proteinâ^'Ligand Complexes. Journal of Proteome Research, 2006, 5, 105-111.	3.7	19
138	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
139	Looking for new xanthine oxidase inhibitors: 3-Phenylcoumarins versus 2-phenylbenzofurans. International Journal of Biological Macromolecules, 2020, 162, 774-780.	7.5	19
140	1,2-Disubstituted cyclohexane nucleosides: comparative study for the synthesis of cis and trans adenosine analogues. Tetrahedron, 2005, 61, 473-478.	1.9	18
141	Stochastic-based descriptors studying biopolymers biological properties: Extended MARCH-INSIDE methodology describing antibacterial activity of lactoferricin derivatives. Biopolymers, 2005, 77, 247-256.	2.4	18
142	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
143	Synthesis, conformational analysis and antiviral and antitumoral activity of new 1,2-disubstituted carbocyclic nucleosides. European Journal of Medicinal Chemistry, 2002, 37, 755-760.	5.5	17
144	New Furan Side Tetracyclic Allopsoralen Derivatives:Â Synthesis and Photobiological Evaluation. Journal of Medicinal Chemistry, 2006, 49, 4317-4326.	6.4	17

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145	Tyrosine-like condensed derivatives as tyrosinase inhibitors. Journal of Pharmacy and Pharmacology, 2012, 64, 742-746.	2.4	16
146	Synthesis and adenosine receptors binding affinities of a series of 3-arylcoumarins. Journal of Pharmacy and Pharmacology, 2013, 65, 1590-1597.	2.4	16
147	Monoamine Oxidase (MAO) Inhibitory Activity: 3â€Phenylcoumarins versus 4â€Hydroxyâ€3â€phenylcoumarins. ChemMedChem, 2014, 9, 1672-1676.	3.2	16
148	3-Arylcoumarins as highly potent and selective monoamine oxidase B inhibitors: Which chemical features matter?. Bioorganic Chemistry, 2020, 101, 103964.	4.1	16
149	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
150	Synthesis and convenient functionalisation of pyridazinofurocoumarins: nitrogenated isosters of potent DNA inhibitors. Tetrahedron, 2003, 59, 8171-8176.	1.9	14
151	A new psoralen derivative with enlarged antiproliferative properties. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 2874-2876.	2.2	14
152	Structure-Based Optimization of Coumarin hA₃ Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2020, 63, 2577-2587.	6.4	14
153	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
154	Synthesis ofCis-1-[(2-Hydroxymethyl) Cyclopentyl]Uridine and Determination of its Conformation by X-Ray Crystallography and Ami Theoretical Calculations. Nucleosides & Nucleotides, 1996, 15, 1179-1187.	0.5	13
155	A slightly shorter route to carbocyclic nucleosides. Synthesis of (Â±)â€transâ€1â€[2â€(hydroxymethyl)cyclopentylmethyl]uracil. Journal of Heterocyclic Chemistry, 1999, 36, 293-295.	2.6	13
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