Milan Randić

List of Publications by Year in descending order

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219 papers 12,635 citations

52 h-index 27406 106 g-index

222 all docs 222 docs citations

times ranked

222

3334 citing authors

#	Article	IF	Citations
1	Graph energy based on the eccentricity matrix. Discrete Mathematics, 2019, 342, 2636-2646.	0.7	25
2	Benzenoid rings resonance energies and local aromaticity of benzenoid hydrocarbons. Journal of Computational Chemistry, 2019, 40, 753-762.	3.3	5
3	Mathematical chemistry illustrations: a personal view of less known results. Journal of Mathematical Chemistry, 2019, 57, 280-314.	1.5	O
4	Aromaticity Revisited. Advances in Quantum Chemistry, 2018, 77, 167-199.	0.8	3
5	The anti-adjacency matrix of a graph: Eccentricity matrix. Discrete Applied Mathematics, 2018, 251, 299-309.	0.9	36
6	Local aromaticity and aromatic sextet theory beyond Clar. International Journal of Quantum Chemistry, 2018, 118, e25657.	2.0	22
7	On Solved and Unsolved Problems in Chemistry. Journal of Computer Chemistry Japan, 2017, 16, 42-46.	0.1	0
8	Protein alignment: Exact versus approximate. An illustration. Journal of Computational Chemistry, 2015, 36, 1069-1074.	3.3	10
9	Novel insight into Clar's aromatic π-sextets. Chemical Physics Letters, 2014, 601, 1-5.	2.6	18
10	Rank of Hadamard powers of Euclidean distance matrices. Journal of Mathematical Chemistry, 2014, 52, 729-740.	1.5	1
11	Canonical labels for protein spots of proteomics maps. Journal of Mathematical Chemistry, 2014, 52, 198-212.	1.5	0
12	On of molecular similarity based on a single molecular descriptor. Chemical Physics Letters, 2014, 599, 1-6.	2.6	9
13	On the centrality of vertices of molecular graphs. Journal of Computational Chemistry, 2013, 34, 2514-2523.	3.3	1
14	Milestones in graphical bioinformatics. International Journal of Quantum Chemistry, 2013, 113, 2413-2446.	2.0	41
15	Very efficient search for nucleotide alignments. Journal of Computational Chemistry, 2013, 34, 77-82.	3.3	10
16	On Map Representations of DNA. Croatica Chemica Acta, 2013, 86, 519-529.	0.4	1
17	Common vertex matrix: A novel characterization of molecular graphs by counting. Journal of Computational Chemistry, 2013, 34, 1409-1419.	3.3	5
18	On characterizing proteomics maps by using weighted Voronoi maps. Journal of Mathematical Chemistry, 2012, 50, 2689-2702.	1.5	4

#	Article	IF	CITATIONS
19	Ï∈-Electron currents in fixed Ï∈-sextet aromatic benzenoids. Journal of Mathematical Chemistry, 2012, 50, 2755-2774.	1.5	10
20	Ï€â€electron currents in polycyclic conjugated hydrocarbons: Coronene and its isomers having five and seven member rings. International Journal of Quantum Chemistry, 2012, 112, 972-985.	2.0	14
21	Ï€â€Electron currents in larger fully aromatic benzenoids. International Journal of Quantum Chemistry, 2012, 112, 2456-2462.	2.0	3
22	Conjugated circuits currents in hexabenzocoronene and its derivatives formed by joining proximal carbons. Journal of Computational Chemistry, 2012, 33, 1111-1122.	3.3	7
23	Applying the conjugated circuits method to Clar structures of [n]phenylenes for determining resonance energies. Physical Chemistry Chemical Physics, 2011, 13, 20644.	2.8	26
24	Graphical Representation of Proteins. Chemical Reviews, 2011, 111, 790-862.	47.7	104
25	Structural Approach to Aromaticity and Local Aromaticity in Conjugated Polycyclic Systems. Carbon Materials, 2011, , 159-204.	1.2	5
26	On numerical characterization of proteomics maps based on partitioning of 2-D maps into Voronoi regions. Journal of Mathematical Chemistry, 2011, 49, 1759-1768.	1.5	4
27	Ï€-Electron Currents in Polycyclic Conjugated Hydrocarbons of Decreasing Aromatic Character and a Novel Structural Definition of Aromaticity#. Open Organic Chemistry Journal, 2011, 5, 11-26.	0.9	24
28	Algebraic clar formulas - numerical representation of clar structural formula. Acta Chimica Slovenica, 2011, 58, 448-57.	0.6	4
29	Novel graph distance matrix. Journal of Computational Chemistry, 2010, 31, 1832-1841.	3.3	9
30	Study of proteome maps using partial ordering. Journal of Theoretical Biology, 2010, 266, 21-28.	1.7	13
31	Graph theoretical approach to π-electron currents in polycyclic conjugated hydrocarbons. Chemical Physics Letters, 2010, 500, 123-127.	2.6	42
32	Use of the Szeged index and the revised Szeged index for measuring network bipartivity. Discrete Applied Mathematics, 2010, 158, 1936-1944.	0.9	59
33	Citations versus limitations of citations: beyond Hirsch index. Scientometrics, 2009, 80, 809-818.	3.0	17
34	Graph theoretical study of structural similarity in benzomorphans. International Journal of Quantum Chemistry, 2009, 16, 55-71.	2.0	2
35	Symmetry properties of graphs of interest in chemistry. III. Homotetrahedryl rearrangement. International Journal of Quantum Chemistry, 2009, 18, 557-577.	2.0	2
36	On intramolecular average ¹³ C chemical shift in nonanes. International Journal of Quantum Chemistry, 2009, 109, 3093-3102.	2.0	0

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37	Spectrumâ€like graphical representation of RNA secondary structure. International Journal of Quantum Chemistry, 2009, 109, 2982-2995.	2.0	7
38	Graphical representation of proteins as four-color maps and their numerical characterization. Journal of Molecular Graphics and Modelling, 2009, 27, 637-641.	2.4	45
39	Novel spectral representation of RNA secondary structure without loss of information. Chemical Physics Letters, 2009, 476, 277-280.	2.6	11
40	On representation of DNA by line distance matrix. Journal of Mathematical Chemistry, 2008, 43, 674-692.	1.5	14
41	On a geometry-based approach to protein sequence alignment. Journal of Mathematical Chemistry, 2008, 43, 756-772.	1.5	17
42	Partition of Ï∈-electrons between faces of polyhedral carbon aggregates. Journal of Mathematical Chemistry, 2008, 43, 773-779.	1.5	8
43	Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. International Journal of Quantum Chemistry, 2008, 108, 898-926.	2.0	12
44	Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. International Journal of Quantum Chemistry, 2008, 108, 865-897.	2.0	14
45	Another look at the chaos-game representation of DNA. Chemical Physics Letters, 2008, 456, 84-88.	2.6	35
46	Correlations between various ways of accounting for the distribution of π-electrons in benzenoids. New Journal of Chemistry, 2008, 32, 1071.	2.8	10
47	New Chessboard (8×8) Representation of the Standard Genetic Code, and Its Application for Representing Primary Structures of Proteins. , 2008, , .		0
48	A New Yardstick for Benzenoid Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2008, 112, 11769-11776.	2.5	5
49	Ï€-Electron Partitions, Signatures, and Clar Structures of Selected Benzenoid Hydrocarbons. Journal of Physical Chemistry A, 2008, 112, 4148-4157.	2.5	13
50	Numerical Kekulé Structures of Fullerenes and Partitioning of π-Electrons to Pentagonal and Hexagonal Rings. Journal of Chemical Information and Modeling, 2007, 47, 897-904.	5.4	22
51	2-D Graphical representation of proteins based on physico-chemical properties of amino acids. Chemical Physics Letters, 2007, 440, 291-295.	2.6	47
52	On representation of proteins by star-like graphs. Journal of Molecular Graphics and Modelling, 2007, 26, 290-305.	2.4	89
53	Partitioning of π-Electrons in Rings for Clar Structures of Benzenoid Hydrocarbons. Journal of Chemical Information and Modeling, 2006, 46, 57-64.	5.4	43
54	Quantitative Characterizations of Proteome:Â Dependence on the Number of Proteins Considered. Journal of Proteome Research, 2006, 5, 1575-1579.	3.7	15

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55	"Anticonnectivity― A Challenge for Structureâ^'Propertyâ^'Activity Studies. Journal of Chemical Information and Modeling, 2006, 46, 2-8.	5.4	15
56	Novel 2-D graphical representation of proteins. Chemical Physics Letters, 2006, 419, 528-532.	2.6	94
57	A novel unexpected use of a graphical representation of DNA: Graphical alignment of DNA sequences. Chemical Physics Letters, 2006, 431, 375-379.	2.6	42
58	On the Dependence of a Characterization of Proteomics Maps on the Number of Protein Spots Considered. Journal of Chemical Information and Modeling, 2006, 46, 116-122.	5.4	13
59	Characterization of Complex Biological Systems by Matrix Invariants. Journal of Computational Biology, 2006, 13, 1558-1564.	1.6	16
60	On Kekulé structures of buckminsterfullerene. Chemical Physics Letters, 2005, 401, 446-450.	2.6	31
61	Four-color map representation of DNA or RNA sequences and their numerical characterization. Chemical Physics Letters, 2005, 407, 205-208.	2.6	52
62	Novel Characterization of Proteomics Maps by Sequential Neighborhoods of Protein Spots. Journal of Chemical Information and Modeling, 2005, 45, 1205-1213.	5.4	20
63	Partitioning of π -electrons in rings of polycyclic conjugated hydrocarbons: Part 6. Comparison with other methods for estimating the local aromaticity of rings in polycyclic benzenoids. Journal of Mathematical Chemistry, 2005, 37, 443-453.	1.5	40
64	Partitioning of ⊨Electrons in Rings of Fibonacenes. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2005, 60, 171-176.	1.5	21
65	Ï€-ELECTRON CONTENTS OF RINGS IN THE DOUBLE-HEXAGONAL-CHAIN HOMOLOGOUS SERIES (PYRENE,) Tj ET	Qq1 _. 1 0.7	′84314 rgBT
66	Algorithm for Coding DNA Sequences into "Spectrum-like―and "Zigzag―Representations. Journal of Chemical Information and Modeling, 2005, 45, 309-313.	5.4	40
67	Canonical Labeling of Proteome Maps. Journal of Proteome Research, 2005, 4, 1347-1352.	3.7	18
68	Order from Chaos:Â Observing Hormesis at the Proteome Level. Journal of Proteome Research, 2005, 4, 2133-2136.	3.7	30
69	Using Variable and Fixed Topological Indices for the Prediction of Reaction Rate Constants of Volatile Unsaturated Hydrocarbons with OH Radicals. Molecules, 2004, 9, 1160-1176.	3.8	28
70	Variable Connectivity Index as a Tool for Modeling Structure-Property Relationships. Molecules, 2004, 9, 1177-1193.	3.8	17
71	Partitioning of Ï€-electrons in Rings of Polycyclic Conjugated Hydrocarbons. Part 4. Benzenoids with More Than One Geometric KekulA© Structure Corresponding to the Same Algebraic Kekulé Structure. Journal of Mathematical Chemistry, 2004, 36, 271-279.	1.5	30
72	ON SIMILARITY OF PROTEOME MAPS. Medicinal Chemistry Research, 2004, 13, 800-811.	2.4	5

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73	Algebraic Kekule Formulas for Benzenoid Hydrocarbons ChemInform, 2004, 35, no.	0.0	O
74	Graphical representations of DNA as 2-D map. Chemical Physics Letters, 2004, 386, 468-471.	2.6	95
75	Unique graphical representation of protein sequences based on nucleotide triplet codons. Chemical Physics Letters, 2004, 397, 247-252.	2.6	97
76	PARTITIONING OF π-ELECTRONS IN RINGS OF POLYCYCLIC conjugated HYDROCARBONS. PART 1: CATACONDENSED BENZENOIDS. Polycyclic Aromatic Compounds, 2004, 24, 173-193.	2.6	55
77	Quantitative characterization of protein structure: application to a novel $\hat{l}\pm/\hat{l}^2$ fold. New Journal of Chemistry, 2004, 28, 1608-1614.	2.8	11
78	Partitioning of Ï€-Electrons in Rings of Polycyclic Conjugated Hydrocarbons. 5. Nonalternant Compoundsâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 1701-1707.	2.8	47
79	Algebraic Kekulé Formulas for Benzenoid Hydrocarbonsâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 365-372.	2.8	50
80	Wienerâ^'Hosoya Index A Novel Graph Theoretical Molecular Descriptorâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 373-377.	2.8	21
81	Algebraic Kekulé Structures of Benzenoid Hydrocarbonsâ€. Journal of Chemical Information and Computer Sciences, 2004, 44, 296-299.	2.8	34
82	Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 3. Perifusenes. New Journal of Chemistry, 2004, 28, 800-806.	2.8	49
83	Partitioning of π-Electrons in Rings of Polycyclic Benzenoid Hydrocarbons. 2.1Catacondensed Coronoids. Journal of Chemical Information and Computer Sciences, 2004, 44, 50-59.	2.8	61
84	On Invariants of a 2-D Proteome Map Derived from Neighborhood Graphs. Journal of Proteome Research, 2004, 3, 778-785.	3.7	19
85	DNA invariants based on nonoverlapping triplets of nucleotide bases. Chemical Physics Letters, 2003, 379, 147-154.	2.6	18
86	Novel 2-D graphical representation of DNA sequences and their numerical characterization. Chemical Physics Letters, 2003, 368, 1-6.	2.6	247
87	Analysis of similarity/dissimilarity of DNA sequences based on novel 2-D graphical representation. Chemical Physics Letters, 2003, 371, 202-207.	2.6	206
88	Compact 2-D graphical representation of DNA. Chemical Physics Letters, 2003, 373, 558-562.	2.6	69
89	Novel map descriptors for characterization of toxic effects in proteomics maps. Journal of Molecular Graphics and Modelling, 2003, 22, 1-9.	2.4	47
90	Characterization of molecular complexity. International Journal of Quantum Chemistry, 2003, 91, 20-31.	2.0	26

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91	Aromaticity of Polycyclic Conjugated Hydrocarbons. Chemical Reviews, 2003, 103, 3449-3606.	47.7	678
92	On a Four-Dimensional Representation of DNA Primary Sequences [J.Chem. Inf. Comput. Sci.43, 532â^539 (2003)]. Journal of Chemical Information and Computer Sciences, 2003, 43, 1724-1724.	2.8	1
93	On A Four-Dimensional Representation of DNA Primary Sequences. Journal of Chemical Information and Computer Sciences, 2003, 43, 532-539.	2.8	117
94	Quantitative Characterization of Proteomics Maps by Matrix Invariants. , 2003, , 429-450.		3
95	Clar's π-aromatic sextet revisited***This paper is honoring Professor Ivan Gutman, a dedicated warrior for a better recognition of Clar's insights into the nature of benzenoids dominate properties of benzenoid systems Theoretical and Computational Chemistry, 2002, , 503-533.	0.4	5
96	On Characterization of Dose Variations of 2-D Proteomics Maps by Matrix Invariants. Journal of Proteome Research, 2002, 1, 217-226.	3.7	32
97	A Comparative Study of Proteomics Maps Using Graph Theoretical Biodescriptors. Journal of Chemical Information and Computer Sciences, 2002, 42, 983-992.	2.8	28
98	A graph theoretical characterization of proteomics maps. International Journal of Quantum Chemistry, 2002, 90, 848-858.	2.0	38
99	Quantum Chemical Justification for Clar's Valence Structures. , 2002, , 204-239.		3
100	On Graphical and Numerical Characterization of Proteomics Maps. Journal of Chemical Information and Computer Sciences, 2001, 41, 1330-1338.	2.8	44
101	On Interpretation of Well-Known Topological Indices. Journal of Chemical Information and Computer Sciences, 2001, 41, 550-560.	2.8	103
102	The Variable Molecular Descriptors Based on Distance Related Matricesâ€. Journal of Chemical Information and Computer Sciences, 2001, 41, 575-581.	2.8	52
103	A New Descriptor for Structureâ^'Property and Structureâ^'Activity Correlationsâ€. Journal of Chemical Information and Computer Sciences, 2001, 41, 650-656.	2.8	39
104	Graph Theoretical Descriptors of Two-Dimensional Chirality with Possible Extension to Three-Dimensional Chirality‡. Journal of Chemical Information and Computer Sciences, 2001, 41, 639-649.	2.8	28
105	On the Characterization of DNA Primary Sequences by Triplet of Nucleic Acid Bases. Journal of Chemical Information and Computer Sciences, 2001, 41, 619-626.	2.8	105
106	The Variable Connectivity Index1χfversus the Traditional Molecular Descriptors:  A Comparative Study of1χfAgainst Descriptors of CODESSA. Journal of Chemical Information and Computer Sciences, 2001, 41, 631-638.	2.8	49
107	On Use of the Variable Connectivity Index1χfin QSAR:  Toxicity of Aliphatic Ethers. Journal of Chemical Information and Computer Sciences, 2001, 41, 614-618.	2.8	76
108	Variable Connectivity Index for Cycle-Containing Structures. Journal of Chemical Information and Computer Sciences, 2001, 41, 657-662.	2.8	63

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109	On 3-D Graphical Representation of Proteomics Maps and Their Numerical Characterization. Journal of Chemical Information and Computer Sciences, 2001, 41, 1339-1344.	2.8	54
110	Retro-RegressionAnother Important Multivariate Regression Improvementâ€. Journal of Chemical Information and Computer Sciences, 2001, 41, 602-606.	2.8	9
111	Novel Shape Descriptors for Molecular Graphs. Journal of Chemical Information and Computer Sciences, 2001, 41, 607-613.	2.8	83
112	On Structural Interpretation of Several Distance Related Topological Indices. Journal of Chemical Information and Computer Sciences, 2001, 41, 593-601.	2.8	42
113	Characterization of DNA Primary Sequences Based on the Average Distances between Bases. Journal of Chemical Information and Computer Sciences, 2001, 41, 561-568.	2.8	40
114	The connectivity index 25 years after. Journal of Molecular Graphics and Modelling, 2001, 20, 19-35.	2.4	198
115	A novel 2-D graphical representation of DNA sequences of low degeneracy. Chemical Physics Letters, 2001, 350, 106-112.	2.6	103
116	Title is missing!. Journal of Mathematical Chemistry, 2001, 30, 325-342.	1.5	2
117	Giant Benzenoid Hydrocarbons. Superphenalene Resonance Energy. Polycyclic Aromatic Compounds, 2000, 18, 49-69.	2.6	2
118	On characterization of physical properties of amino acids. International Journal of Quantum Chemistry, 2000, 80, 1199-1209.	2.0	43
119	On characterization of DNA primary sequences by a condensed matrix. Chemical Physics Letters, 2000, 317, 29-34.	2.6	60
120	Proposal for Using an Untapped Source of Citations Characterizing Scientific Areas. Scientometrics, 2000, 49, 517-521.	3.0	0
121	About one - an inquiry about the meanings and uses of the number one. International Journal of Mathematical Education in Science and Technology, 2000, 31, 811-824.	1.4	3
122	High quality structure–property regressions. Boiling points of smaller alkanes. New Journal of Chemistry, 2000, 24, 165-171.	2.8	26
123	On the Similarity of DNA Primary Sequences. Journal of Chemical Information and Computer Sciences, 2000, 40, 599-606.	2.8	112
124	Condensed Representation of DNA Primary Sequences. Journal of Chemical Information and Computer Sciences, 2000, 40, 50-56.	2.8	93
125	Construction of High-Quality Structureâ^'Propertyâ^'Activity Regressions:  The Boiling Points of Sulfides. Journal of Chemical Information and Computer Sciences, 2000, 40, 899-905.	2.8	35
126	Use of path matrices for a characterization of molecular structures. DIMACS Series in Discrete Mathematics and Theoretical Computer Science, 2000, , 305-322.	0.0	9

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127	Resonance energy of giant benzenoid hydrocarbon C78H26. International Journal of Quantum Chemistry, 1999, 74, 697-708.	2.0	9
128	On a characterization of the folding of proteins. International Journal of Quantum Chemistry, 1999, 75, 1017-1026.	2.0	55
129	Optimal Molecular Descriptors Based on Weighted Path Numbers. Journal of Chemical Information and Computer Sciences, 1999, 39, 261-266.	2.8	73
130	On structural ordering and branching of acyclic saturated hydrocarbons. Journal of Mathematical Chemistry, 1998, 24, 345-358.	1.5	21
131	Optimal molecular connectivity descriptors for nitrogen-containing molecules. International Journal of Quantum Chemistry, 1998, 70, 1209-1215.	2.0	42
132	Clar Polynomials of Large Benzenoid Systems. Journal of Chemical Information and Computer Sciences, 1998, 38, 563-574.	2.8	12
133	Much ado about nothing—an introductive inquiry about zero. International Journal of Mathematical Education in Science and Technology, 1998, 29, 729-744.	1.4	7
134	Dense Graphs and Sparse Matrices. Journal of Chemical Information and Computer Sciences, 1997, 37, 1078-1081.	2.8	14
135	On Characterization of Cyclic Structures. Journal of Chemical Information and Computer Sciences, 1997, 37, 1063-1071.	2.8	38
136	On Characterization of Chemical Structure. Journal of Chemical Information and Computer Sciences, 1997, 37, 672-687.	2.8	165
137	Hierarchical orthogonalization of descriptors. International Journal of Quantum Chemistry, 1997, 63, 215-222.	2.0	58
138	Resonance in catacondensed benzenoid hydrocarbons. International Journal of Quantum Chemistry, 1997, 63, 585-600.	2.0	34
139	On characterization of molecular surfaces. International Journal of Quantum Chemistry, 1997, 65, 1065-1076.	2.0	22
140	Characterization of 3-D sequences of proteins. Chemical Physics Letters, 1997, 272, 115-119.	2.6	46
141	Orthosimilarity. Journal of Chemical Information and Computer Sciences, 1996, 36, 1092-1097.	2.8	12
142	Bond profiles for cuboctahedron and twist cuboctahedron. International Journal of Quantum Chemistry, 1996, 60, 1851-1863.	2.0	6
143	Higher-order Fibonacci numbers. Journal of Mathematical Chemistry, 1996, 20, 79-94.	1.5	18
144	Molecular bonding profiles. Journal of Mathematical Chemistry, 1996, 19, 375-392.	1.5	38

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145	On characterization of the conformations of nine-membered rings. International Journal of Quantum Chemistry, 1995, 56, 61-73.	2.0	11
146	On Construction of Clar Structures for Large Benzenoids. Polycyclic Aromatic Compounds, 1995, 4, 249-269.	2.6	13
147	On Characterization of Molecular Shapes. Journal of Chemical Information and Computer Sciences, 1995, 35, 594-606.	2.8	28
148	Molecular Shape Profiles. Journal of Chemical Information and Computer Sciences, 1995, 35, 373-382.	2.8	70
149	Compact Codes: On Nomenclature of Acyclic Chemical Compounds. Journal of Chemical Information and Computer Sciences, 1995, 35, 357-365.	2.8	8
150	Restricted random walks on graphs. Theoretica Chimica Acta, 1995, 92, 97-106.	0.8	17
151	On the Characterization of Fullerenes. Fullerenes, Nanotubes, and Carbon Nanostructures, 1994, 2, 427-444.	0.6	4
152	Generalized bond orders. International Journal of Quantum Chemistry, 1994, 49, 215-237.	2.0	7
153	On conjugated-circuit polynomials. International Journal of Quantum Chemistry, 1994, 50, 369-384.	2.0	8
154	Curve-fitting paradox. International Journal of Quantum Chemistry, 1994, 52, 215-225.	2.0	7
155	Distance/Distance Matrixes. Journal of Chemical Information and Computer Sciences, 1994, 34, 277-286.	2.8	119
156	Novel molecular descriptor for structureâ€"property studies. Chemical Physics Letters, 1993, 211, 478-483.	2.6	273
157	Fitting of nonlinear regressions by orthogonalized power series. Journal of Computational Chemistry, 1993, 14, 363-370.	3.3	47
158	Representation of molecular graphs by basic graphs. Journal of Chemical Information and Computer Sciences, 1992, 32, 57-69.	2.8	35
159	In search of structural invariants. Journal of Mathematical Chemistry, 1992, 9, 97-146.	1.5	56
160	Resolution of ambiguities in structure-property studies by use of orthogonal descriptors. Journal of Chemical Information and Computer Sciences, 1991, 31, 311-320.	2.8	223
161	On the Relative Stability of Nonbenzenoid Alternant Hydrocarbons. Polycyclic Aromatic Compounds, 1991, 2, 183-194.	2.6	8
162	Novel graph theoretical approach to heteroatoms in quantitative structureâ€"activity relationships. Chemometrics and Intelligent Laboratory Systems, 1991, 10, 213-227.	3.5	122

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163	Correlation of enthalphy of octanes with orthogonal connectivity indices. Computational and Theoretical Chemistry, 1991, 233, 45-59.	1.5	100
164	On computation of optimal parameters for multivariate analysis of structure-property relationship. Journal of Computational Chemistry, 1991, 12, 970-980.	3.3	111
165	Computer-assisted studies of structure-property relationships using graph invariants. Magnetic Resonance in Chemistry, 1991, 29, 362-365.	1.9	7
166	On the difference in bond orders betweenHMO andPPP methods. International Journal of Quantum Chemistry, 1990, 37, 437-448.	2.0	10
167	On a Fragment Approach to Structure-activity Correlations. QSAR and Combinatorial Science, 1989, 8, 39-48.	1.2	16
168	On the construction of the matching polynomial for unbranched catacondensed benzenoids. Journal of Computational Chemistry, 1989, 10, 683-697.	3.3	17
169	The conjugated-circuit model: application to benzenoid hydrocarbons. Journal of Molecular Structure, 1989, 198, 223-237.	3.6	39
170	Computer assisted structure-taste studies on sulfamates by pattern recognition method using graph theoretical invariants. Journal of Computational Chemistry, 1988, 9, 636-646.	3.3	20
171	Composition as a method for data reduction: application to carbon-13 NMR chemical shifts. Theoretica Chimica Acta, 1988, 73, 233-246.	0.8	24
172	On characterization of three-dimensional structures. International Journal of Quantum Chemistry, 1988, 34, 201-208.	2.0	45
173	A rational selection of graph-theoretical indices in the QSAR. International Journal of Quantum Chemistry, 1988, 34, 267-285.	2.0	18
174	Conjugation and aromaticity of macrocyclic systems. International Journal of Quantum Chemistry, 1988, 34, 127-141.	2.0	13
175	Clar's valence structures of benzenoid hydrocarbons. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 1875.	1.1	13
176	Resonance energies of large conjugated hydrocarbons by a statistical method. International Journal of Quantum Chemistry, 1987, 32, 35-59.	2.0	18
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178	On the evaluation of the characteristic polynomial via symmetric function theory. Journal of Mathematical Chemistry, 1987, 1, 145-152.	1.5	43
179	Graph generators. Journal of Computational Chemistry, 1987, 8, 522-535.	3.3	8
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182	A graph theoretical approach to Mi; $^{1/2}$ bius systems in organic chemistry. International Journal of Quantum Chemistry, 1986, 30, 185-201.	2.0	10
183	On the stability of conjugated hydrocarbon ions. International Journal of Quantum Chemistry, 1986, 30, 203-218.	2.0	6
184	On some solved and unsolved problems of chemical graph theory. International Journal of Quantum Chemistry, 1986, 30, 699-742.	2.0	42
185	On irreducible endospectral graphs. Journal of Mathematical Physics, 1986, 27, 2601-2612.	1.1	24
186	A graph theoretical approach to quantitative structure-activity relationship. International Journal of Quantum Chemistry, 1985, 28, 123-139.	2.0	4
187	On molecular identification numbers. Journal of Chemical Information and Computer Sciences, 1984, 24, 164-175.	2.8	191
188	Symmetry properties of chemical graphs. VI. Isomerizations of octahedral complexes. International Journal of Quantum Chemistry, 1984, 26, 69-89.	2.0	19
189	Nonempirical approach to structure-activity studies. International Journal of Quantum Chemistry, 1984, 26, 137-153.	2.0	47
190	Conjugation and aromaticity of corannulenes. Journal of the American Chemical Society, 1984, 106, 4428-4434.	13.7	72
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193	Symmetry properties of chemical graphs. V. Internal rotation inXY?3XY?2XY3. Journal of Computational Chemistry, 1983, 4, 73-83.	3.3	6
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196	The graph center concept for polycyclic graphs. International Journal of Quantum Chemistry, 1981, 19, 61-82.	2.0	33
197	Resonance energy of very large benzenoid hydrocarbons. International Journal of Quantum Chemistry, 1980, 17, 549-586.	2.0	70
198	Graphâ€theoretical analysis of molecular properties. Isomeric variations in nonanes. International Journal of Quantum Chemistry, 1980, 18, 1005-1027.	2.0	30

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