Milan Randic

List of Publications by Year in Descending Order

218 papers	10,806 citations	48 h-index	98 g-index
222 ext. papers	11,613 ext. citations	3.6 avg, IF	6.66 L-index

#	Paper	IF	Citations
218	Graph energy based on the eccentricity matrix. *Discrete Mathematics*, **2019**, 342, 2636-2646	0.7	13
217	Benzenoid rings resonance energies and local aromaticity of benzenoid hydrocarbons. *Journal of Computational Chemistry*, **2019**, 40, 753-762	3.5	3
216	Mathematical chemistry illustrations: a personal view of less known results. *Journal of Mathematical Chemistry*, **2019**, 57, 280-314	2.1	
215	The anti-adjacency matrix of a graph: Eccentricity matrix. *Discrete Applied Mathematics*, **2018**, 251, 299-309	1.9	20
214	Local aromaticity and aromatic sextet theory beyond Clar. *International Journal of Quantum Chemistry*, **2018**, 118, e25657	2.1	13
213	Aromaticity Revisited. *Advances in Quantum Chemistry*, **2018**, 77, 167-199	1.4	3
212	On Solved and Unsolved Problems in Chemistry. *Journal of Computer Chemistry Japan*, **2017**, 16, 42-46	0.2	
211	Protein alignment: Exact versus approximate. An illustration. *Journal of Computational Chemistry*, **2015**, 36, 1069-74	3.5	9
210	On of molecular similarity based on a single molecular descriptor. *Chemical Physics Letters*, **2014**, 599, 1-6	2.5	6
209	Novel insight into Clar's aromatic sextets. *Chemical Physics Letters*, **2014**, 601, 1-5	2.5	17
208	Rank of Hadamard powers of Euclidean distance matrices. *Journal of Mathematical Chemistry*, **2014**, 52, 729-740	2.1	1
207	Canonical labels for protein spots of proteomics maps. *Journal of Mathematical Chemistry*, **2014**, 52, 198-212	2.1	
206	On the centrality of vertices of molecular graphs. *Journal of Computational Chemistry*, **2013**, 34, 2514-23	3.5	
205	Milestones in graphical bioinformatics. *International Journal of Quantum Chemistry*, **2013**, 113, 2413-2446	2.1	26
204	Very efficient search for nucleotide alignments. *Journal of Computational Chemistry*, **2013**, 34, 77-82	3.5	10
203	On Map Representations of DNA. *Croatica Chemica Acta*, **2013**, 86, 519-529	0.8	0
202	Common vertex matrix: a novel characterization of molecular graphs by counting. *Journal of Computational Chemistry*, **2013**, 34, 1409-19	3.5	3

201	On characterizing proteomics maps by using weighted Voronoi maps. *Journal of Mathematical Chemistry*, **2012**, 50, 2689-2702	2.1	3
200	Electron currents in fixed sextet aromatic benzenoids. *Journal of Mathematical Chemistry*, **2012**, 50, 2755-2774	2.1	9
199	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	2.1	12
198	Electron currents in larger fully aromatic benzenoids. *International Journal of Quantum Chemistry*, **2012**, 112, 2456-2462	2.1	3
197	Conjugated circuits currents in hexabenzocoronene and its derivatives formed by joining proximal carbons. *Journal of Computational Chemistry*, **2012**, 33, 1111-22	3.5	7
196	Structural Approach to Aromaticity and Local Aromaticity in Conjugated Polycyclic Systems. *Carbon Materials*, **2011**, 159-204		4
195	On numerical characterization of proteomics maps based on partitioning of 2-D maps into Voronoi regions. *Journal of Mathematical Chemistry*, **2011**, 49, 1759-1768	2.1	4
194	Applying the conjugated circuits method to Clar structures of [n]phenylenes for determining resonance energies. *Physical Chemistry Chemical Physics*, **2011**, 13, 20644-8	3.6	21
193	Graphical representation of proteins. *Chemical Reviews*, **2011**, 111, 790-862	68.1	88
192	Management of post laser in situ keratomileusis ectasia with simultaneous topography guided photorefractive keratectomy and collagen cross-linking. *Open Organic Chemistry Journal*, **2011**, 5, 11-3		19
191	Detailed Atlas of Kekul Structures of the Buckminsterfullerene. *Carbon Materials*, **2011**, 153-169		1
190	Algebraic clar formulas - numerical representation of clar structural formula. *Acta Chimica Slovenica* , **2011**, 58, 448-57	1.9	4
189	Novel graph distance matrix. *Journal of Computational Chemistry*, **2010**, 31, 1832-41	3.5	4
188	Study of proteome maps using partial ordering. *Journal of Theoretical Biology*, **2010**, 266, 21-8	2.3	11
187	Graph theoretical approach to electron currents in polycyclic conjugated hydrocarbons. *Chemical Physics Letters*, **2010**, 500, 123-127	2.5	39
186	Use of the Szeged index and the revised Szeged index for measuring network bipartivity. *Discrete Applied Mathematics*, **2010**, 158, 1936-1944	1	49
185	Citations versus limitations of citations: beyond Hirsch index. *Scientometrics*, **2009**, 80, 809-818	3	11
184	Graph-theoretical analysis of structure-property and structure-activity correlations. *International Journal of Quantum Chemistry*, **2009**, 14, 245-255	2.1	17

183	Graph theoretical study of structural similarity in benzomorphans. *International Journal of Quantum Chemistry*, **2009**, 16, 55-71	2.1	
182	Graphical enumeration of conformations of chains. *International Journal of Quantum Chemistry*, **2009**, 18, 187-197	2.1	1
181	Symmetry properties of graphs of interest in chemistry. III. Homotetrahedryl rearrangement. *International Journal of Quantum Chemistry*, **2009**, 18, 557-577	2.1	
180	A graph theoretical approach to quantitative structure-activity relationship. *International Journal of Quantum Chemistry*, **2009**, 28, 123-139	2.1	1
179	On intramolecular average 13C chemical shift in nonanes. *International Journal of Quantum Chemistry*, **2009**, 109, 3093-3102	2.1	
178	Spectrum-like graphical representation of RNA secondary structure. *International Journal of Quantum Chemistry*, **2009**, 109, 2982-2995	2.1	7
177	Graphical representation of proteins as four-color maps and their numerical characterization. *Journal of Molecular Graphics and Modelling*, **2009**, 27, 637-41	2.8	41
176	Novel spectral representation of RNA secondary structure without loss of information. *Chemical Physics Letters*, **2009**, 476, 277-280	2.5	11
175	Correlations between various ways of accounting for the distribution of π-electrons in benzenoids. *New Journal of Chemistry*, **2008**, 32, 1071	3.6	10
174	A new yardstick for benzenoid polycyclic aromatic hydrocarbons. *Journal of Physical Chemistry A*, **2008**, 112, 11769-76	2.8	5
173	Pi-electron partitions, signatures, and Clar structures of selected benzenoid hydrocarbons. *Journal of Physical Chemistry A*, **2008**, 112, 4148-57	2.8	12
172	On representation of DNA by line distance matrix. *Journal of Mathematical Chemistry*, **2008**, 43, 674-692	2.1	12
171	On a geometry-based approach to protein sequence alignment. *Journal of Mathematical Chemistry*, **2008**, 43, 756-772	2.1	17
170	Partition of π-electrons between faces of polyhedral carbon aggregates. *Journal of Mathematical Chemistry*, **2008**, 43, 773-779	2.1	8
169	Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. *International Journal of Quantum Chemistry*, **2008**, 108, 898-926	2.1	12
168	Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. *International Journal of Quantum Chemistry*, **2008**, 108, 865-897	2.1	13
167	Another look at the chaos-game representation of DNA. *Chemical Physics Letters*, **2008**, 456, 84-88	2.5	29
166	Numerical Kekulé structures of fullerenes and partitioning of pi-electrons to pentagonal and hexagonal rings. *Journal of Chemical Information and Modeling*, **2007**, 47, 897-904	6.1	20

165	2-D Graphical representation of proteins based on physico-chemical properties of amino acids. *Chemical Physics Letters*, **2007**, 440, 291-295	2.5	45
164	On representation of proteins by star-like graphs. *Journal of Molecular Graphics and Modelling*, **2007**, 26, 290-305	2.8	78
163	Characterization of complex biological systems by matrix invariants. *Journal of Computational Biology*, **2006**, 13, 1558-64	1.7	14
162	Partitioning of pi-electrons in rings for Clar structures of benzenoid hydrocarbons. *Journal of Chemical Information and Modeling*, **2006**, 46, 57-64	6.1	38
161	Quantitative characterizations of proteome: dependence on the number of proteins considered. *Journal of Proteome Research*, **2006**, 5, 1575-9	5.6	12
160	"Anticonnectivity": a challenge for structure-property-activity studies. *Journal of Chemical Information and Modeling*, **2006**, 46, 2-8	6.1	8
159	Novel 2-D graphical representation of proteins. *Chemical Physics Letters*, **2006**, 419, 528-532	2.5	86
158	A novel unexpected use of a graphical representation of DNA: Graphical alignment of DNA sequences. *Chemical Physics Letters*, **2006**, 431, 375-379	2.5	36
157	On the dependence of a characterization of proteomics maps on the number of protein spots considered. *Journal of Chemical Information and Modeling*, **2006**, 46, 116-22	6.1	9
156	Algorithm for coding DNA sequences into "spectrum-like" and "zigzag" representations. *Journal of Chemical Information and Modeling*, **2005**, 45, 309-13	6.1	36
155	Canonical labeling of proteome maps. *Journal of Proteome Research*, **2005**, 4, 1347-52	5.6	15
154	Order from chaos: observing hormesis at the proteome level. *Journal of Proteome Research*, **2005**, 4, 2133-6	5.6	29
153	On Kekul□structures of buckminsterfullerene. *Chemical Physics Letters*, **2005**, 401, 446-450	2.5	25
152	Four-color map representation of DNA or RNA sequences and their numerical characterization. *Chemical Physics Letters*, **2005**, 407, 205-208	2.5	41
151	Novel characterization of proteomics maps by sequential neighborhoods of protein spots. *Journal of Chemical Information and Modeling*, **2005**, 45, 1205-13	6.1	15
150	Partitioning of □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	2.1	40
149	Partitioning of □Electrons in Rings of Fibonacenes. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2005**, 60, 171-176	1.4	20
148	□ELECTRON CONTENTS OF RINGS IN THE DOUBLE-HEXAGONAL-CHAIN HOMOLOGOUS SERIES (PYRENE, ANTHANTHRENE AND OTHER ACENOACENES). *Polycyclic Aromatic Compounds*, **2005**, 25, 215-226	1.3	15

147	Using variable and fixed topological indices for the prediction of reaction rate constants of volatile unsaturated hydrocarbons with OH radicals. *Molecules*, **2004**, 9, 1160-76	4.8	21
146	Variable connectivity index as a tool for modeling structure-property relationships. *Molecules*, **2004**, 9, 1177-93	4.8	11
145	Partitioning of π-electrons in Rings of Polycyclic Conjugated Hydrocarbons. Part 4. Benzenoids with More Than One Geometric Kekulé Structure Corresponding to the Same Algebraic Kekulé Structure. *Journal of Mathematical Chemistry*, **2004**, 36, 271-279	2.1	30
144	ON SIMILARITY OF PROTEOME MAPS. *Medicinal Chemistry Research*, **2004**, 13, 800-811	2.2	4
143	Graphical representations of DNA as 2-D map. *Chemical Physics Letters*, **2004**, 386, 468-471	2.5	79
142	Unique graphical representation of protein sequences based on nucleotide triplet codons. *Chemical Physics Letters*, **2004**, 397, 247-252	2.5	83
141	PARTITIONING OF π-ELECTRONS IN RINGS OF POLYCYCLIC conjugated HYDROCARBONS. PART 1: CATACONDENSED BENZENOIDS. *Polycyclic Aromatic Compounds*, **2004**, 24, 173-193	1.3	49
140	Quantitative characterization of protein structure: application to a novel β-fold. *New Journal of Chemistry*, **2004**, 28, 1608-1614	3.6	9
139	Partitioning of pi-electrons in rings of polycyclic conjugated hydrocarbons. 5. Nonalternant compounds. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 1701-7		45
138	Algebraic Kekulé formulas for benzenoid hydrocarbons. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 365-72		48
137	Wiener-Hosoya index--a novel graph theoretical molecular descriptor. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 373-7		19
136	Algebraic Kekulé structures of benzenoid hydrocarbons. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 296-9		31
135	Partitioning of π-electrons in rings of polycyclic conjugated hydrocarbons. Part 3. Perifusenes. *New Journal of Chemistry*, **2004**, 28, 800-806	3.6	47
134	Partitioning of pi-electrons in rings of polycyclic benzenoid hydrocarbons. 2.1. Catacondensed coronoids. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 50-9		55
133	On invariants of a 2-D proteome map derived from neighborhood graphs. *Journal of Proteome Research*, **2004**, 3, 778-85	5.6	16
132	DNA invariants based on nonoverlapping triplets of nucleotide bases. *Chemical Physics Letters*, **2003**, 379, 147-154	2.5	15
131	Novel 2-D graphical representation of DNA sequences and their numerical characterization. *Chemical Physics Letters*, **2003**, 368, 1-6	2.5	211
130	Analysis of similarity/dissimilarity of DNA sequences based on novel 2-D graphical representation. *Chemical Physics Letters*, **2003**, 371, 202-207	2.5	180

129	Compact 2-D graphical representation of DNA. *Chemical Physics Letters*, **2003**, 373, 558-562	2.5	60
128	Novel map descriptors for characterization of toxic effects in proteomics maps. *Journal of Molecular Graphics and Modelling*, **2003**, 22, 1-9	2.8	37
127	Characterization of molecular complexity. *International Journal of Quantum Chemistry*, **2003**, 91, 20-31	2.1	15
126	Aromaticity of polycyclic conjugated hydrocarbons. *Chemical Reviews*, **2003**, 103, 3449-605	68.1	584
125	On a Four-Dimensional Representation of DNA Primary Sequences [J. Chem. Inf. Comput. Sci. 43, 532□39 (2003)]. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1724-1724		
124	On a four-dimensional representation of DNA primary sequences. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 532-9		98
123	Quantitative Characterization of Proteomics Maps by Matrix Invariants **2003**, 429-450		3
122	A graph theoretical characterization of proteomics maps. *International Journal of Quantum Chemistry*, **2002**, 90, 848-858	2.1	29
121	Clar□ □aromatic sextet revisited***This paper is honoring Professor Ivan Gutman, a dedicated warrior for a better recognition of Clar□ insights into the nature of benzenoids dominate properties of benzenoid systems.. *Theoretical and Computational Chemistry*, **2002**, 503-533		5
120	On characterization of dose variations of 2-D proteomics maps by matrix invariants. *Journal of Proteome Research*, **2002**, 1, 217-26	5.6	26
119	A comparative study of proteomics maps using graph theoretical biodescriptors. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 983-92		23
118	Quantum Chemical Justification for Clar□ Valence Structures **2002**, 204-239		3
117	Characterization of DNA primary sequences based on the average distances between bases. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 561-8		36
116	The connectivity index 25 years after. *Journal of Molecular Graphics and Modelling*, **2001**, 20, 19-35	2.8	158
115	A novel 2-D graphical representation of DNA sequences of low degeneracy. *Chemical Physics Letters* , **2001**, 350, 106-112	2.5	88
114	Recursive Formulae for Enumeration of LM-Conjugated Circuits in Structurally Related Benzenoid Hydrocarbons. *Journal of Mathematical Chemistry*, **2001**, 30, 325-342	2.1	2
113	On graphical and numerical characterization of proteomics maps. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1330-8		39
112	On interpretation of well-known topological indices. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 550-60		85

111	The variable molecular descriptors based on distance related matrices. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 575-81		45
110	A new descriptor for structure-property and structure-activity correlations. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 650-6		31
109	Graph theoretical descriptors of two-dimensional chirality with possible extension to three-dimensional chirality. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 639-49		21
108	On the characterization of DNA primary sequences by triplet of nucleic acid bases. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 619-26		96
107	The variable connectivity index 1chi(f) versus the traditional molecular descriptors: a comparative study of 1chi(f) against descriptors of CODESSA. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 631-8		43
106	On use of the variable connectivity index 1chi(f) in QSAR: toxicity of aliphatic ethers. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 614-8		63
105	Variable connectivity index for cycle-containing structures. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 657-62		48
104	On 3-D graphical representation of proteomics maps and their numerical characterization. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1339-44		50
103	Retro-regression--another important multivariate regression improvement. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 602-6		7
102	Novel shape descriptors for molecular graphs. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 607-13		73
101	On structural interpretation of several distance related topological indices. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 593-601		32
100	Giant Benzenoid Hydrocarbons. Superphenalene Resonance Energy. *Polycyclic Aromatic Compounds* , **2000**, 18, 49-69	1.3	1
99	On characterization of physical properties of amino acids. *International Journal of Quantum Chemistry*, **2000**, 80, 1199-1209	2.1	39
98	On characterization of DNA primary sequences by a condensed matrix. *Chemical Physics Letters*, **2000**, 317, 29-34	2.5	54
97	Proposal for Using an Untapped Source of Citations Characterizing Scientific Areas. *Scientometrics*, **2000**, 49, 517-521	3	
96	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	0.5	1
95	High quality structure–property regressions. Boiling points of smaller alkanes. *New Journal of Chemistry*, **2000**, 24, 165-171	3.6	24
94	On the similarity of DNA primary sequences. *Journal of Chemical Information and Computer Sciences* , **2000**, 40, 599-606		99

93	Condensed representation of DNA primary sequences. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 50-6		84
92	Construction of high-quality structure-property-activity regressions: the boiling points of sulfides. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 899-905		32
91	Use of path matrices for a characterization of molecular structures. *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, **2000**, 305-322		8
90	Resonance energy of giant benzenoid hydrocarbon C78H26. *International Journal of Quantum Chemistry*, **1999**, 74, 697-708	2.1	8
89	On a characterization of the folding of proteins. *International Journal of Quantum Chemistry*, **1999**, 75, 1017-1026	2.1	48
88	Optimal Molecular Descriptors Based on Weighted Path Numbers. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 261-266		62
87	On structural ordering and branching of acyclic saturated hydrocarbons. *Journal of Mathematical Chemistry*, **1998**, 24, 345-358	2.1	18
86	Optimal molecular connectivity descriptors for nitrogen-containing molecules. *International Journal of Quantum Chemistry*, **1998**, 70, 1209-1215	2.1	36
85	Clar Polynomials of Large Benzenoid Systems. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 563-574		8
84	Much ado about nothing□n introductive inquiry about zero. *International Journal of Mathematical Education in Science and Technology*, **1998**, 29, 729-744	0.5	5
83	Dense Graphs and Sparse Matrices. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 1078-1081		12
82	On Characterization of Cyclic Structures. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 1063-1071		31
81	On Characterization of Chemical Structure. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 672-687		149
80	Hierarchical orthogonalization of descriptors. *International Journal of Quantum Chemistry*, **1997**, 63, 215-222	2.1	48
79	Resonance in catacondensed benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, **1997**, 63, 585-600	2.1	29
78	On characterization of molecular surfaces. *International Journal of Quantum Chemistry*, **1997**, 65, 1065-1076	2.1	19
77	Characterization of 3-D sequences of proteins. *Chemical Physics Letters*, **1997**, 272, 115-119	2.5	43
76	Orthosimilarity. *Journal of Chemical Information and Computer Sciences*, **1996**, 36, 1092-1097		8

75	Bond profiles for cuboctahedron and twist cuboctahedron. *International Journal of Quantum Chemistry*, **1996**, 60, 1851-1863	2.1	5
74	Higher-order Fibonacci numbers. *Journal of Mathematical Chemistry*, **1996**, 20, 79-94	2.1	15
73	Molecular bonding profiles. *Journal of Mathematical Chemistry*, **1996**, 19, 375-392	2.1	31
72	On characterization of the conformations of nine-membered rings. *International Journal of Quantum Chemistry*, **1995**, 56, 61-73	2.1	9
71	On Construction of Clar Structures for Large Benzenoids. *Polycyclic Aromatic Compounds*, **1995**, 4, 249-269	0.3	12
70	On Characterization of Molecular Shapes. *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 594-606		26
69	Molecular Shape Profiles. *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 373-382		61
68	Compact Codes: On Nomenclature of Acyclic Chemical Compounds. *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 357-365		7
67	Restricted random walks on graphs. *Theoretica Chimica Acta*, **1995**, 92, 97-106		13
66	On the Characterization of Fullerenes. *Fullerenes, Nanotubes, and Carbon Nanostructures*, **1994**, 2, 427-444		3
65	Generalized bond orders. *International Journal of Quantum Chemistry*, **1994**, 49, 215-237	2.1	4
64	On conjugated circuit polynomials. *International Journal of Quantum Chemistry*, **1994**, 50, 369-384	2.1	7
63	Curve-fitting paradox. *International Journal of Quantum Chemistry*, **1994**, 52, 215-225	2.1	2
62	Distance/Distance Matrixes. *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 277-286		100
61	Novel molecular descriptor for structure property studies. *Chemical Physics Letters*, **1993**, 211, 478-483	2.5	219
60	Fitting of nonlinear regressions by orthogonalized power series. *Journal of Computational Chemistry*, **1993**, 14, 363-370	3.5	42
59	Representation of molecular graphs by basic graphs. *Journal of Chemical Information and Computer Sciences*, **1992**, 32, 57-69		28
58	In search of structural invariants. *Journal of Mathematical Chemistry*, **1992**, 9, 97-146	2.1	48

57	On the Relative Stability of Nonbenzenoid Alternant Hydrocarbons. *Polycyclic Aromatic Compounds*, **1991**, 2, 183-194	1.3	7
56	Novel graph theoretical approach to heteroatoms in quantitative structure–activity relationships. *Chemometrics and Intelligent Laboratory Systems*, **1991**, 10, 213-227	3.8	106
55	Correlation of enthalphy of octanes with orthogonal connectivity indices. *Computational and Theoretical Chemistry*, **1991**, 233, 45-59		92
54	On computation of optimal parameters for multivariate analysis of structure-property relationship. *Journal of Computational Chemistry*, **1991**, 12, 970-980	3.5	94
53	Computer-assisted studies of structure–property relationships using graph invariants. *Magnetic Resonance in Chemistry*, **1991**, 29, 362-365	2.1	6
52	Resolution of ambiguities in structure-property studies by use of orthogonal descriptors. *Journal of Chemical Information and Computer Sciences*, **1991**, 31, 311-320		199
51	On the difference in bond orders between HMO and PPP methods. *International Journal of Quantum Chemistry*, **1990**, 37, 437-448	2.1	8
50	On a Fragment Approach to Structure-activity Correlations. *QSAR and Combinatorial Science*, **1989**, 8, 39-48		13
49	On the construction of the matching polynomial for unbranched catacondensed benzenoids. *Journal of Computational Chemistry*, **1989**, 10, 683-697	3.5	15
48	The conjugated-circuit model: application to benzenoid hydrocarbons. *Journal of Molecular Structure*, **1989**, 198, 223-237	3.4	36
47	Computer assisted structure–taste studies on sulfamates by pattern recognition method using graph theoretical invariants. *Journal of Computational Chemistry*, **1988**, 9, 636-646	3.5	18
46	Composition as a method for data reduction: application to carbon-13 NMR chemical shifts. *Theoretica Chimica Acta*, **1988**, 73, 233-246		17
45	On characterization of three-dimensional structures. *International Journal of Quantum Chemistry*, **1988**, 34, 201-208	2.1	41
44	A rational selection of graph-theoretical indices in the QSAR. *International Journal of Quantum Chemistry*, **1988**, 34, 267-285	2.1	15
43	Conjugation and aromaticity of macrocyclic systems. *International Journal of Quantum Chemistry*, **1988**, 34, 127-141	2.1	12
42	Clar's valence structures of benzenoid hydrocarbons. *Journal of the Chemical Society, Faraday Transactions 2*, **1988**, 84, 1875		12
41	Resonance energies of large conjugated hydrocarbons by a statistical method. *International Journal of Quantum Chemistry*, **1987**, 32, 35-59	2.1	18
40	The search for active substructures in structure-activity studies. *International Journal of Quantum Chemistry*, **1987**, 32, 245-260	2.1	1

39	On the evaluation of the characteristic polynomial via symmetric function theory. *Journal of Mathematical Chemistry*, **1987**, 1, 145-152	2.1	38
38	Graph generators. *Journal of Computational Chemistry*, **1987**, 8, 522-535	3.5	6
37	On the Relative Stabilities of Conjugated Heterocycles Containing Divalent Sulfur. *Sulfur Reports*, **1986**, 6, 379-426		9
36	Symmetry properties of chemical graphs. IX. The valence tautomerism in the P73□skeleton. *Journal of Computational Chemistry*, **1986**, 7, 35-54	3.5	26
35	A graph theoretical approach to M□bius systems in organic chemistry. *International Journal of Quantum Chemistry*, **1986**, 30, 185-201	2.1	10
34	On the stability of conjugated hydrocarbon ions. *International Journal of Quantum Chemistry*, **1986**, 30, 203-218	2.1	6
33	On some solved and unsolved problems of chemical graph theory. *International Journal of Quantum Chemistry*, **1986**, 30, 699-742	2.1	35
32	On irreducible endospectral graphs. *Journal of Mathematical Physics*, **1986**, 27, 2601-2612	1.2	18
31	On molecular identification numbers. *Journal of Chemical Information and Computer Sciences*, **1984**, 24, 164-175		164
30	Symmetry properties of chemical graphs. VI. Isomerizations of octahedral complexes. *International Journal of Quantum Chemistry*, **1984**, 26, 69-89	2.1	13
29	Nonempirical approach to structure□ctivity studies. *International Journal of Quantum Chemistry*, **1984**, 26, 137-153	2.1	41
28	Conjugation and aromaticity of corannulenes. *Journal of the American Chemical Society*, **1984**, 106, 4428-4434	10.4	67
27	Survey of structural regularities in molecular properties. I. Carbon-13 chemical shifts in alkanes. *International Journal of Quantum Chemistry*, **1983**, 23, 1707-1722	2.1	22
26	Unusual random walks. *International Journal of Quantum Chemistry*, **1983**, 24, 435-452	2.1	16
25	Symmetry properties of chemical graphs. V. Internal rotation in XY?3XY?2XY3. *Journal of Computational Chemistry*, **1983**, 4, 73-83	3.5	6
24	On evaluation of the characteristic polynomial for large molecules. *Journal of Computational Chemistry*, **1982**, 3, 421-435	3.5	43
23	Symmetry properties of chemical graphs. IV. Rearrangement of tetragonal-pyramidal complexes. *International Journal of Quantum Chemistry*, **1982**, 21, 647-663	2.1	15
22	The graph center concept for polycyclic graphs. *International Journal of Quantum Chemistry*, **1981**, 19, 61-82	2.1	28

21	Resonance energy of very large benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, **1980**, 17, 549-586	2.1	66
20	Graph-theoretical analysis of molecular properties. Isomeric variations in nonanes. *International Journal of Quantum Chemistry*, **1980**, 18, 1005-1027	2.1	29
19	Random walks and their diagnostic value for characterization of atomic environment. *Journal of Computational Chemistry*, **1980**, 1, 386-399	3.5	87
18	A correlation between Kekul valence structures and conjugated circuits. *Chemical Physics*, **1979**, 41, 265-270	2.3	51
17	Symmetry properties of graphs of interest in chemistry. II. Desargues levi graph. *International Journal of Quantum Chemistry*, **1979**, 15, 663-682	2.1	39
16	Graph theoretical ordering of structures as a basis for systematic searches for regularities in molecular data. *The Journal of Physical Chemistry*, **1979**, 83, 1525-1540		99
15	On a graph theoretical basis for ordering of structures. *Chemical Physics Letters*, **1979**, 63, 332-336	2.5	58
14	On the parity of Kekul structures. *Molecular Physics*, **1977**, 34, 849-856	1.7	29
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