

# Milan RandiÄ

## List of Publications by Year in descending order

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219  
papers

12,635  
citations

34105

52  
h-index

27406

106  
g-index

222  
all docs

222  
docs citations

222  
times ranked

3334  
citing authors

#	ARTICLE	IF	CITATIONS
1	Characterization of molecular branching. Journal of the American Chemical Society, 1975, 97, 6609-6615.	13.7	2,810
2	Aromaticity of Polycyclic Conjugated Hydrocarbons. Chemical Reviews, 2003, 103, 3449-3606.	47.7	678
3	Aromaticity and conjugation. Journal of the American Chemical Society, 1977, 99, 444-450.	13.7	386
4	Conjugated circuits and resonance energies of benzenoid hydrocarbons. Chemical Physics Letters, 1976, 38, 68-70.	2.6	295
5	Novel molecular descriptor for structureâ€™property studies. Chemical Physics Letters, 1993, 211, 478-483.	2.6	273
6	Novel 2-D graphical representation of DNA sequences and their numerical characterization. Chemical Physics Letters, 2003, 368, 1-6.	2.6	247
7	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
8	Analysis of similarity/dissimilarity of DNA sequences based on novel 2-D graphical representation. Chemical Physics Letters, 2003, 371, 202-207.	2.6	206
9	The connectivity index 25 years after. Journal of Molecular Graphics and Modelling, 2001, 20, 19-35.	2.4	198
10	Molecular Connectivity V: Connectivity Series Concept Applied to Density. Journal of Pharmaceutical Sciences, 1976, 65, 1226-1230.	3.3	194
11	On molecular identification numbers. Journal of Chemical Information and Computer Sciences, 1984, 24, 164-175.	2.8	191
12	A graph theoretical approach to conjugation and resonance energies of hydrocarbons. Tetrahedron, 1977, 33, 1905-1920.	1.9	190
13	On Characterization of Chemical Structure. Journal of Chemical Information and Computer Sciences, 1997, 37, 672-687.	2.8	165
14	On the recognition of identical graphs representing molecular topology. Journal of Chemical Physics, 1974, 60, 3920-3928.	3.0	132
15	Novel graph theoretical approach to heteroatoms in quantitative structureâ€™activity relationships. Chemometrics and Intelligent Laboratory Systems, 1991, 10, 213-227.	3.5	122
16	Distance/Distance Matrixes. Journal of Chemical Information and Computer Sciences, 1994, 34, 277-286.	2.8	119
17	On A Four-Dimensional Representation of DNA Primary Sequences. Journal of Chemical Information and Computer Sciences, 2003, 43, 532-539.	2.8	117
18	On the Similarity of DNA Primary Sequences. Journal of Chemical Information and Computer Sciences, 2000, 40, 599-606.	2.8	112

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19	On computation of optimal parameters for multivariate analysis of structure-property relationship. <i>Journal of Computational Chemistry</i> , 1991, 12, 970-980.	3.3	111
20	Graph theoretical ordering of structures as a basis for systematic searches for regularities in molecular data. <i>The Journal of Physical Chemistry</i> , 1979, 83, 1525-1540.	2.9	108
21	On the Characterization of DNA Primary Sequences by Triplet of Nucleic Acid Bases. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 619-626.	2.8	105
22	Graphical Representation of Proteins. <i>Chemical Reviews</i> , 2011, 111, 790-862.	47.7	104
23	On Interpretation of Well-Known Topological Indices. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 550-560.	2.8	103
24	A novel 2-D graphical representation of DNA sequences of low degeneracy. <i>Chemical Physics Letters</i> , 2001, 350, 106-112.	2.6	103
25	Correlation of enthalpy of octanes with orthogonal connectivity indices. <i>Computational and Theoretical Chemistry</i> , 1991, 233, 45-59.	1.5	100
26	Unique graphical representation of protein sequences based on nucleotide triplet codons. <i>Chemical Physics Letters</i> , 2004, 397, 247-252.	2.6	97
27	Random walks and their diagnostic value for characterization of atomic environment. <i>Journal of Computational Chemistry</i> , 1980, 1, 386-399.	3.3	96
28	Graphical representations of DNA as 2-D map. <i>Chemical Physics Letters</i> , 2004, 386, 468-471.	2.6	95
29	Novel 2-D graphical representation of proteins. <i>Chemical Physics Letters</i> , 2006, 419, 528-532.	2.6	94
30	Condensed Representation of DNA Primary Sequences. <i>Journal of Chemical Information and Computer Sciences</i> , 2000, 40, 50-56.	2.8	93
31	On representation of proteins by star-like graphs. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 290-305.	2.4	89
32	Novel Shape Descriptors for Molecular Graphs. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 607-613.	2.8	83
33	On Use of the Variable Connectivity Index in QSAR: Toxicity of Aliphatic Ethers. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 614-618.	2.8	76
34	Optimal Molecular Descriptors Based on Weighted Path Numbers. <i>Journal of Chemical Information and Computer Sciences</i> , 1999, 39, 261-266.	2.8	73
35	Enumeration of the Kekulé structures in conjugated hydrocarbons. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1976, 72, 232-243.	1.1	72
36	Conjugation and aromaticity of corannulenes. <i>Journal of the American Chemical Society</i> , 1984, 106, 4428-4434.	13.7	72

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37	On Canonical Numbering of Atoms in a Molecule and Graph Isomorphism. <i>Journal of Chemical Information and Modeling</i> , 1977, 17, 171-180.	5.4	70
38	Resonance energy of very large benzenoid hydrocarbons. <i>International Journal of Quantum Chemistry</i> , 1980, 17, 549-586.	2.0	70
39	Molecular Shape Profiles. <i>Journal of Chemical Information and Computer Sciences</i> , 1995, 35, 373-382.	2.8	70
40	Compact 2-D graphical representation of DNA. <i>Chemical Physics Letters</i> , 2003, 373, 558-562.	2.6	69
41	On a graph theoretical basis for ordering of structures. <i>Chemical Physics Letters</i> , 1979, 63, 332-336.	2.6	64
42	Variable Connectivity Index for Cycle-Containing Structures. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 657-662.	2.8	63
43	Partitioning of $\pi$ -Electrons in Rings of Polycyclic Benzenoid Hydrocarbons. 2.1 Catacondensed Coronoids. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 50-59.	2.8	61
44	On characterization of DNA primary sequences by a condensed matrix. <i>Chemical Physics Letters</i> , 2000, 317, 29-34.	2.6	60
45	Use of the Szeged index and the revised Szeged index for measuring network bipartivity. <i>Discrete Applied Mathematics</i> , 2010, 158, 1936-1944.	0.9	59
46	Hierarchical orthogonalization of descriptors. <i>International Journal of Quantum Chemistry</i> , 1997, 63, 215-222.	2.0	58
47	In search of structural invariants. <i>Journal of Mathematical Chemistry</i> , 1992, 9, 97-146.	1.5	56
48	On a characterization of the folding of proteins. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 1017-1026.	2.0	55
49	PARTITIONING OF $\pi$ -ELECTRONS IN RINGS OF POLYCYCLIC conjugated HYDROCARBONS. PART 1: CATACONDENSED BENZENOIDS. <i>Polycyclic Aromatic Compounds</i> , 2004, 24, 173-193.	2.6	55
50	On 3-D Graphical Representation of Proteomics Maps and Their Numerical Characterization. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 1339-1344.	2.8	54
51	A correlation between Kekulé valence structures and conjugated circuits. <i>Chemical Physics</i> , 1979, 41, 265-270.	1.9	53
52	On evaluation of the characteristic polynomial for large molecules. <i>Journal of Computational Chemistry</i> , 1982, 3, 421-435.	3.3	52
53	The Variable Molecular Descriptors Based on Distance Related Matrices. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 575-581.	2.8	52
54	Four-color map representation of DNA or RNA sequences and their numerical characterization. <i>Chemical Physics Letters</i> , 2005, 407, 205-208.	2.6	52

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55	Algebraic Kekulé Formulas for Benzenoid Hydrocarbons. Journal of Chemical Information and Computer Sciences, 2004, 44, 365-372.	2.8	50
56	The Variable Connectivity Index versus the Traditional Molecular Descriptors: A Comparative Study of Against Descriptors of CODESSA. Journal of Chemical Information and Computer Sciences, 2001, 41, 631-638.	2.8	49
57	Partitioning of $\pi$ -electrons in rings of polycyclic conjugated hydrocarbons. Part 3. Perifusenes. New Journal of Chemistry, 2004, 28, 800-806.	2.8	49
58	Nonempirical approach to structure-activity studies. International Journal of Quantum Chemistry, 1984, 26, 137-153.	2.0	47
59	Fitting of nonlinear regressions by orthogonalized power series. Journal of Computational Chemistry, 1993, 14, 363-370.	3.3	47
60	Novel map descriptors for characterization of toxic effects in proteomics maps. Journal of Molecular Graphics and Modelling, 2003, 22, 1-9.	2.4	47
61	Partitioning of $\pi$ -Electrons in Rings of Polycyclic Conjugated Hydrocarbons. 5. Nonalternant Compounds. Journal of Chemical Information and Computer Sciences, 2004, 44, 1701-1707.	2.8	47
62	2-D Graphical representation of proteins based on physico-chemical properties of amino acids. Chemical Physics Letters, 2007, 440, 291-295.	2.6	47
63	Characterization of 3-D sequences of proteins. Chemical Physics Letters, 1997, 272, 115-119.	2.6	46
64	On characterization of three-dimensional structures. International Journal of Quantum Chemistry, 1988, 34, 201-208.	2.0	45
65	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
66	On Unique Numbering of Atoms and Unique Codes for Molecular Graphs. Journal of Chemical Information and Modeling, 1975, 15, 105-108.	5.4	44
67	On Graphical and Numerical Characterization of Proteomics Maps. Journal of Chemical Information and Computer Sciences, 2001, 41, 1330-1338.	2.8	44
68	Symmetry properties of graphs of interest in chemistry. II. Desargues-Levi graph. International Journal of Quantum Chemistry, 1979, 15, 663-682.	2.0	43
69	On the evaluation of the characteristic polynomial via symmetric function theory. Journal of Mathematical Chemistry, 1987, 1, 145-152.	1.5	43
70	On characterization of physical properties of amino acids. International Journal of Quantum Chemistry, 2000, 80, 1199-1209.	2.0	43
71	Partitioning of $\pi$ -Electrons in Rings for Clar Structures of Benzenoid Hydrocarbons. Journal of Chemical Information and Modeling, 2006, 46, 57-64.	5.4	43
72	On some solved and unsolved problems of chemical graph theory. International Journal of Quantum Chemistry, 1986, 30, 699-742.	2.0	42

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73	Optimal molecular connectivity descriptors for nitrogen-containing molecules. <i>International Journal of Quantum Chemistry</i> , 1998, 70, 1209-1215.	2.0	42
74	On Structural Interpretation of Several Distance Related Topological Indices. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 593-601.	2.8	42
75	A novel unexpected use of a graphical representation of DNA: Graphical alignment of DNA sequences. <i>Chemical Physics Letters</i> , 2006, 431, 375-379.	2.6	42
76	Graph theoretical approach to $\pi$ -electron currents in polycyclic conjugated hydrocarbons. <i>Chemical Physics Letters</i> , 2010, 500, 123-127.	2.6	42
77	Milestones in graphical bioinformatics. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 2413-2446.	2.0	41
78	Characterization of DNA Primary Sequences Based on the Average Distances between Bases. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 561-568.	2.8	40
79	Partitioning of $\pi$ -electrons in rings of polycyclic conjugated hydrocarbons: Part 6. Comparison with other methods for estimating the local aromaticity of rings in polycyclic benzenoids. <i>Journal of Mathematical Chemistry</i> , 2005, 37, 443-453.	1.5	40
80	Algorithm for Coding DNA Sequences into "Spectrum-like" and "Zigzag" Representations. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 309-313.	5.4	40
81	The conjugated-circuit model: application to benzenoid hydrocarbons. <i>Journal of Molecular Structure</i> , 1989, 198, 223-237.	3.6	39
82	A New Descriptor for Structure~Property and Structure~Activity Correlations. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 650-656.	2.8	39
83	Molecular bonding profiles. <i>Journal of Mathematical Chemistry</i> , 1996, 19, 375-392.	1.5	38
84	On Characterization of Cyclic Structures. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 1063-1071.	2.8	38
85	A graph theoretical characterization of proteomics maps. <i>International Journal of Quantum Chemistry</i> , 2002, 90, 848-858.	2.0	38
86	The anti-adjacency matrix of a graph: Eccentricity matrix. <i>Discrete Applied Mathematics</i> , 2018, 251, 299-309.	0.9	36
87	Representation of molecular graphs by basic graphs. <i>Journal of Chemical Information and Computer Sciences</i> , 1992, 32, 57-69.	2.8	35
88	Construction of High-Quality Structure~Property~Activity Regressions: The Boiling Points of Sulfides. <i>Journal of Chemical Information and Computer Sciences</i> , 2000, 40, 899-905.	2.8	35
89	Another look at the chaos-game representation of DNA. <i>Chemical Physics Letters</i> , 2008, 456, 84-88.	2.6	35
90	Resonance in catacondensed benzenoid hydrocarbons. <i>International Journal of Quantum Chemistry</i> , 1997, 63, 585-600.	2.0	34

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91	Algebraic Kekulé Structures of Benzenoid Hydrocarbons. Journal of Chemical Information and Computer Sciences, 2004, 44, 296-299.	2.8	34
92	The graph center concept for polycyclic graphs. International Journal of Quantum Chemistry, 1981, 19, 61-82.	2.0	33
93	On Characterization of Dose Variations of 2-D Proteomics Maps by Matrix Invariants. Journal of Proteome Research, 2002, 1, 217-226.	3.7	32
94	Symmetry properties of chemical graphs. IX. The valence tautomerism in the P73? skeleton. Journal of Computational Chemistry, 1986, 7, 35-54.	3.3	31
95	On Kekulé structures of buckminsterfullerene. Chemical Physics Letters, 2005, 401, 446-450.	2.6	31
96	Graph-theoretical analysis of molecular properties. Isomeric variations in nonanes. International Journal of Quantum Chemistry, 1980, 18, 1005-1027.	2.0	30
97	Partitioning of $\pi$ -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.	1.5	30
98	Order from Chaos: Observing Hormesis at the Proteome Level. Journal of Proteome Research, 2005, 4, 2133-2136.	3.7	30
99	Solved and Unsolved Problems of Structural Chemistry. , 0, , .		30
100	On the parity of Kekulé structures. Molecular Physics, 1977, 34, 849-856.	1.7	29
101	On Characterization of Molecular Shapes. Journal of Chemical Information and Computer Sciences, 1995, 35, 594-606.	2.8	28
102	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
103	A Comparative Study of Proteomics Maps Using Graph Theoretical Biodescriptors. Journal of Chemical Information and Computer Sciences, 2002, 42, 983-992.	2.8	28
104	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
105	High quality structure-property regressions. Boiling points of smaller alkanes. New Journal of Chemistry, 2000, 24, 165-171.	2.8	26
106	Characterization of molecular complexity. International Journal of Quantum Chemistry, 2003, 91, 20-31.	2.0	26
107	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
108	Graph energy based on the eccentricity matrix. Discrete Mathematics, 2019, 342, 2636-2646.	0.7	25

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109	On irreducible endospectral graphs. <i>Journal of Mathematical Physics</i> , 1986, 27, 2601-2612.	1.1	24
110	Composition as a method for data reduction: application to carbon-13 NMR chemical shifts. <i>Theoretica Chimica Acta</i> , 1988, 73, 233-246.	0.8	24
111	π-Electron Currents in Polycyclic Conjugated Hydrocarbons of Decreasing Aromatic Character and a Novel Structural Definition of Aromaticity#. <i>Open Organic Chemistry Journal</i> , 2011, 5, 11-26.	0.9	24
112	Survey of structural regularities in molecular properties. I. Carbon-13 chemical shifts in alkanes. <i>International Journal of Quantum Chemistry</i> , 1983, 23, 1707-1722.	2.0	23
113	Unusual random walks. <i>International Journal of Quantum Chemistry</i> , 1983, 24, 435-452.	2.0	22
114	On characterization of molecular surfaces. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 1065-1076.	2.0	22
115	Numerical Kekulé Structures of Fullerenes and Partitioning of π-Electrons to Pentagonal and Hexagonal Rings. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 897-904.	5.4	22
116	Local aromaticity and aromatic sextet theory beyond Clar. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25657.	2.0	22
117	On rearrangement of the connectivity matrix of a graph. <i>Journal of Chemical Physics</i> , 1975, 62, 309.	3.0	21
118	On structural ordering and branching of acyclic saturated hydrocarbons. <i>Journal of Mathematical Chemistry</i> , 1998, 24, 345-358.	1.5	21
119	Wiener's Hosoya Index A Novel Graph Theoretical Molecular Descriptor. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 373-377.	2.8	21
120	Partitioning of π-Electrons in Rings of Fibonacenes. <i>Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences</i> , 2005, 60, 171-176.	1.5	21
121	Computer assisted structure-taste studies on sulfamates by pattern recognition method using graph theoretical invariants. <i>Journal of Computational Chemistry</i> , 1988, 9, 636-646.	3.3	20
122	Novel Characterization of Proteomics Maps by Sequential Neighborhoods of Protein Spots. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 1205-1213.	5.4	20
123	Symmetry properties of chemical graphs. VI. Isomerizations of octahedral complexes. <i>International Journal of Quantum Chemistry</i> , 1984, 26, 69-89.	2.0	19
124	On Invariants of a 2-D Proteome Map Derived from Neighborhood Graphs. <i>Journal of Proteome Research</i> , 2004, 3, 778-785.	3.7	19
125	Resonance energies of large conjugated hydrocarbons by a statistical method. <i>International Journal of Quantum Chemistry</i> , 1987, 32, 35-59.	2.0	18
126	A rational selection of graph-theoretical indices in the QSAR. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 267-285.	2.0	18



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127	Higher-order Fibonacci numbers. <i>Journal of Mathematical Chemistry</i> , 1996, 20, 79-94.	1.5	18
128	DNA invariants based on nonoverlapping triplets of nucleotide bases. <i>Chemical Physics Letters</i> , 2003, 379, 147-154.	2.6	18
129	Canonical Labeling of Proteome Maps. <i>Journal of Proteome Research</i> , 2005, 4, 1347-1352.	3.7	18
130	Graph-theoretical analysis of structure-property and structure-activity correlations. <i>International Journal of Quantum Chemistry</i> , 1978, 14, 245-255.	2.0	18
131	Novel insight into Clar's aromatic sextets. <i>Chemical Physics Letters</i> , 2014, 601, 1-5.	2.6	18
132	On the construction of the matching polynomial for unbranched catacondensed benzenoids. <i>Journal of Computational Chemistry</i> , 1989, 10, 683-697.	3.3	17
133	Restricted random walks on graphs. <i>Theoretica Chimica Acta</i> , 1995, 92, 97-106.	0.8	17
134	Variable Connectivity Index as a Tool for Modeling Structure-Property Relationships. <i>Molecules</i> , 2004, 9, 1177-1193.	3.8	17
135	On a geometry-based approach to protein sequence alignment. <i>Journal of Mathematical Chemistry</i> , 2008, 43, 756-772.	1.5	17
136	Citations versus limitations of citations: beyond Hirsch index. <i>Scientometrics</i> , 2009, 80, 809-818.	3.0	17
137	Symmetry properties of chemical graphs. IV. Rearrangement of tetragonal-pyramidal complexes. <i>International Journal of Quantum Chemistry</i> , 1982, 21, 647-663.	2.0	16
138	On a Fragment Approach to Structure-activity Correlations. <i>QSAR and Combinatorial Science</i> , 1989, 8, 39-48.	1.2	16
139	π-ELECTRON CONTENTS OF RINGS IN THE DOUBLE-HEXAGONAL-CHAIN HOMOLOGOUS SERIES (PYRENE,) $T_j$ $ETQ_{11}$ 0.784314 $rgB_{16}$	2.6	16
140	Characterization of Complex Biological Systems by Matrix Invariants. <i>Journal of Computational Biology</i> , 2006, 13, 1558-1564.	1.6	16
141	Quantitative Characterizations of Proteome: Dependence on the Number of Proteins Considered. <i>Journal of Proteome Research</i> , 2006, 5, 1575-1579.	3.7	15
142	Anticonnectivity: A Challenge for Structure-Property-Activity Studies. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 2-8.	5.4	15
143	Dense Graphs and Sparse Matrices. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 1078-1081.	2.8	14
144	On representation of DNA by line distance matrix. <i>Journal of Mathematical Chemistry</i> , 2008, 43, 674-692.	1.5	14

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145	Ring signatures for benzenoids with up to seven rings, Part 1: Catacondensed systems. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 865-897.	2.0	14
146	π-Electron currents in polycyclic conjugated hydrocarbons: Coronene and its isomers having five and seven member rings. <i>International Journal of Quantum Chemistry</i> , 2012, 112, 972-985.	2.0	14
147	Conjugation and aromaticity of macrocyclic systems. <i>International Journal of Quantum Chemistry</i> , 1988, 34, 127-141.	2.0	13
148	Clar's valence structures of benzenoid hydrocarbons. <i>Journal of the Chemical Society, Faraday Transactions 2</i> , 1988, 84, 1875.	1.1	13
149	On Construction of Clar Structures for Large Benzenoids. <i>Polycyclic Aromatic Compounds</i> , 1995, 4, 249-269.	2.6	13
150	On the Dependence of a Characterization of Proteomics Maps on the Number of Protein Spots Considered. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 116-122.	5.4	13
151	π-Electron Partitions, Signatures, and Clar Structures of Selected Benzenoid Hydrocarbons. <i>Journal of Physical Chemistry A</i> , 2008, 112, 4148-4157.	2.5	13
152	Study of proteome maps using partial ordering. <i>Journal of Theoretical Biology</i> , 2010, 266, 21-28.	1.7	13
153	Orthosimilarity. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 1092-1097.	2.8	12
154	Clar Polynomials of Large Benzenoid Systems. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 563-574.	2.8	12
155	Ring signatures for benzenoids with up to seven rings, Part 2: Pericondensed systems. <i>International Journal of Quantum Chemistry</i> , 2008, 108, 898-926.	2.0	12
156	On characterization of the conformations of nine-membered rings. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 61-73.	2.0	11
157	Quantitative characterization of protein structure: application to a novel $\hat{\alpha}/\hat{\beta}^2$ fold. <i>New Journal of Chemistry</i> , 2004, 28, 1608-1614.	2.8	11
158	Novel spectral representation of RNA secondary structure without loss of information. <i>Chemical Physics Letters</i> , 2009, 476, 277-280.	2.6	11
159	A graph theoretical approach to $M_{1/2}$ systems in organic chemistry. <i>International Journal of Quantum Chemistry</i> , 1986, 30, 185-201.	2.0	10
160	On the difference in bond orders between HMO and PPP methods. <i>International Journal of Quantum Chemistry</i> , 1990, 37, 437-448.	2.0	10
161	Correlations between various ways of accounting for the distribution of π-electrons in benzenoids. <i>New Journal of Chemistry</i> , 2008, 32, 1071.	2.8	10
162	π-Electron currents in fixed π-sextet aromatic benzenoids. <i>Journal of Mathematical Chemistry</i> , 2012, 50, 2755-2774.	1.5	10

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163	Very efficient search for nucleotide alignments. <i>Journal of Computational Chemistry</i> , 2013, 34, 77-82.	3.3	10
164	Protein alignment: Exact versus approximate. An illustration. <i>Journal of Computational Chemistry</i> , 2015, 36, 1069-1074.	3.3	10
165	On the Relative Stabilities of Conjugated Heterocycles Containing Divalent Sulfur. <i>Sulfur Reports</i> , 1986, 6, 379-426.	0.4	9
166	Resonance energy of giant benzenoid hydrocarbon C <sub>78</sub> H <sub>26</sub> . <i>International Journal of Quantum Chemistry</i> , 1999, 74, 697-708.	2.0	9
167	Retro-Regression Another Important Multivariate Regression Improvement. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 602-606.	2.8	9
168	Novel graph distance matrix. <i>Journal of Computational Chemistry</i> , 2010, 31, 1832-1841.	3.3	9
169	On of molecular similarity based on a single molecular descriptor. <i>Chemical Physics Letters</i> , 2014, 599, 1-6.	2.6	9
170	Use of path matrices for a characterization of molecular structures. <i>DIMACS Series in Discrete Mathematics and Theoretical Computer Science</i> , 2000, , 305-322.	0.0	9
171	Graph generators. <i>Journal of Computational Chemistry</i> , 1987, 8, 522-535.	3.3	8
172	On the Relative Stability of Nonbenzenoid Alternant Hydrocarbons. <i>Polycyclic Aromatic Compounds</i> , 1991, 2, 183-194.	2.6	8
173	On conjugated-circuit polynomials. <i>International Journal of Quantum Chemistry</i> , 1994, 50, 369-384.	2.0	8
174	Compact Codes: On Nomenclature of Acyclic Chemical Compounds. <i>Journal of Chemical Information and Computer Sciences</i> , 1995, 35, 357-365.	2.8	8
175	Partition of $\pi$ -electrons between faces of polyhedral carbon aggregates. <i>Journal of Mathematical Chemistry</i> , 2008, 43, 773-779.	1.5	8
176	Hybridization by the maximum overlap method. <i>International Journal of Quantum Chemistry</i> , 1974, 8, 643-676.	2.0	7
177	Computer-assisted studies of structure-property relationships using graph invariants. <i>Magnetic Resonance in Chemistry</i> , 1991, 29, 362-365.	1.9	7
178	Generalized bond orders. <i>International Journal of Quantum Chemistry</i> , 1994, 49, 215-237.	2.0	7
179	Curve-fitting paradox. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 215-225.	2.0	7
180	Much ado about nothing – an introductive inquiry about zero. <i>International Journal of Mathematical Education in Science and Technology</i> , 1998, 29, 729-744.	1.4	7

#	ARTICLE	IF	CITATIONS
181	Spectrum-like graphical representation of RNA secondary structure. International Journal of Quantum Chemistry, 2009, 109, 2982-2995.	2.0	7
182	Conjugated circuits currents in hexabenzocoronene and its derivatives formed by joining proximal carbons. Journal of Computational Chemistry, 2012, 33, 1111-1122.	3.3	7
183	Symmetry properties of chemical graphs. V. Internal rotation in XY <sub>3</sub> XY <sub>2</sub> XY <sub>3</sub> . Journal of Computational Chemistry, 1983, 4, 73-83.	3.3	6
184	On the stability of conjugated hydrocarbon ions. International Journal of Quantum Chemistry, 1986, 30, 203-218.	2.0	6
185	Bond profiles for cuboctahedron and twist cuboctahedron. International Journal of Quantum Chemistry, 1996, 60, 1851-1863.	2.0	6
186	The search for active substructures in structure-activity studies. International Journal of Quantum Chemistry, 1987, 32, 245-260.	2.0	5
187	Clar's $\pi$ -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
188	ON SIMILARITY OF PROTEOME MAPS. Medicinal Chemistry Research, 2004, 13, 800-811.	2.4	5
189	A New Yardstick for Benzenoid Polycyclic Aromatic Hydrocarbons. Journal of Physical Chemistry A, 2008, 112, 11769-11776.	2.5	5
190	Structural Approach to Aromaticity and Local Aromaticity in Conjugated Polycyclic Systems. Carbon Materials, 2011, , 159-204.	1.2	5
191	Common vertex matrix: A novel characterization of molecular graphs by counting. Journal of Computational Chemistry, 2013, 34, 1409-1419.	3.3	5
192	Benzenoid rings resonance energies and local aromaticity of benzenoid hydrocarbons. Journal of Computational Chemistry, 2019, 40, 753-762.	3.3	5
193	Quantitative Characterization of Proteomics Maps by Matrix Invariants. , 0, , 429-450.		5
194	On the Characterization of Fullerenes. Fullerenes, Nanotubes, and Carbon Nanostructures, 1994, 2, 427-444.	0.6	4
195	A graph theoretical approach to quantitative structure-activity relationship. International Journal of Quantum Chemistry, 1985, 28, 123-139.	2.0	4
196	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
197	On characterizing proteomics maps by using weighted Voronoi maps. Journal of Mathematical Chemistry, 2012, 50, 2689-2702.	1.5	4
198	Algebraic clar formulas - numerical representation of clar structural formula. Acta Chimica Slovenica, 2011, 58, 448-57.	0.6	4

#	ARTICLE	IF	CITATIONS
199	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
200	Electron currents in larger fully aromatic benzenoids. International Journal of Quantum Chemistry, 2012, 112, 2456-2462.	2.0	3
201	Aromaticity Revisited. Advances in Quantum Chemistry, 2018, 77, 167-199.	0.8	3
202	Quantitative Characterization of Proteomics Maps by Matrix Invariants. , 2003, , 429-450.		3
203	Quantum Chemical Justification for Clar's Valence Structures. , 2002, , 204-239.		3
204	Giant Benzenoid Hydrocarbons. Superphenalene Resonance Energy. Polycyclic Aromatic Compounds, 2000, 18, 49-69.	2.6	2
205	Title is missing!. Journal of Mathematical Chemistry, 2001, 30, 325-342.	1.5	2
206	Graph theoretical study of structural similarity in benzomorphans. International Journal of Quantum Chemistry, 2009, 16, 55-71.	2.0	2
207	Graphical enumeration of conformations of chains. International Journal of Quantum Chemistry, 1980, 18, 187-197.	2.0	2
208	Symmetry properties of graphs of interest in chemistry. III. Homotetrahydryl rearrangement. International Journal of Quantum Chemistry, 2009, 18, 557-577.	2.0	2
209	On a Four-Dimensional Representation of DNA Primary Sequences [J.Chem. Inf. Comput. Sci.43, 532-539 (2003)]. Journal of Chemical Information and Computer Sciences, 2003, 43, 1724-1724.	2.8	1
210	On the centrality of vertices of molecular graphs. Journal of Computational Chemistry, 2013, 34, 2514-2523.	3.3	1
211	On Map Representations of DNA. Croatica Chemica Acta, 2013, 86, 519-529.	0.4	1
212	Rank of Hadamard powers of Euclidean distance matrices. Journal of Mathematical Chemistry, 2014, 52, 729-740.	1.5	1
213	Proposal for Using an Untapped Source of Citations Characterizing Scientific Areas. Scientometrics, 2000, 49, 517-521.	3.0	0
214	Algebraic Kekule Formulas for Benzenoid Hydrocarbons.. ChemInform, 2004, 35, no.	0.0	0
215	New Chessboard (8x8) Representation of the Standard Genetic Code, and Its Application for Representing Primary Structures of Proteins. , 2008, , .		0
216	On intramolecular average <sup>13</sup> C chemical shift in nonanes. International Journal of Quantum Chemistry, 2009, 109, 3093-3102.	2.0	0

#	ARTICLE	IF	CITATIONS
217	Canonical labels for protein spots of proteomics maps. Journal of Mathematical Chemistry, 2014, 52, 198-212.	1.5	0
218	On Solved and Unsolved Problems in Chemistry. Journal of Computer Chemistry Japan, 2017, 16, 42-46.	0.1	0
219	Mathematical chemistry illustrations: a personal view of less known results. Journal of Mathematical Chemistry, 2019, 57, 280-314.	1.5	0