Milan Randic

List of Publications by Citations

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	Characterization of molecular branching. *Journal of the American Chemical Society*, **1975**, 97, 6609-6615	16.4	2324
217	Aromaticity of polycyclic conjugated hydrocarbons. *Chemical Reviews*, **2003**, 103, 3449-605	68.1	584
216	Aromaticity and conjugation. *Journal of the American Chemical Society*, **1977**, 99, 444-450	16.4	345
215	Conjugated circuits and resonance energies of benzenoid hydrocarbons. *Chemical Physics Letters*, **1976**, 38, 68-70	2.5	273
214	Novel molecular descriptor for structure□property studies. *Chemical Physics Letters*, **1993**, 211, 478-483	2.5	219
213	Novel 2-D graphical representation of DNA sequences and their numerical characterization. *Chemical Physics Letters*, **2003**, 368, 1-6	2.5	211
212	Resolution of ambiguities in structure-property studies by use of orthogonal descriptors. *Journal of Chemical Information and Computer Sciences*, **1991**, 31, 311-320		199
211	Analysis of similarity/dissimilarity of DNA sequences based on novel 2-D graphical representation. *Chemical Physics Letters*, **2003**, 371, 202-207	2.5	180
210	A graph theoretical approach to conjugation and resonance energies of hydrocarbons. *Tetrahedron*, **1977**, 33, 1905-1920	2.4	177
209	Molecular connectivity V: connectivity series concept applied to density. *Journal of Pharmaceutical Sciences*, **1976**, 65, 1226-30	3.9	168
208	On molecular identification numbers. *Journal of Chemical Information and Computer Sciences*, **1984**, 24, 164-175		164
207	The connectivity index 25 years after. *Journal of Molecular Graphics and Modelling*, **2001**, 20, 19-35	2.8	158
206	On Characterization of Chemical Structure. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 672-687		149
205	On the recognition of identical graphs representing molecular topology. *Journal of Chemical Physics* , **1974**, 60, 3920-3928	3.9	111
204	Novel graph theoretical approach to heteroatoms in quantitative structure□ctivity relationships. *Chemometrics and Intelligent Laboratory Systems*, **1991**, 10, 213-227	3.8	106
203	Distance/Distance Matrixes. *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 277-286		100
202	On the similarity of DNA primary sequences. *Journal of Chemical Information and Computer Sciences* , **2000**, 40, 599-606		99

201	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
200	On a four-dimensional representation of DNA primary sequences. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 532-9		98
199	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
198	On computation of optimal parameters for multivariate analysis of structure-property relationship. *Journal of Computational Chemistry*, **1991**, 12, 970-980	3.5	94
197	Correlation of enthalphy of octanes with orthogonal connectivity indices. *Computational and Theoretical Chemistry*, **1991**, 233, 45-59		92
196	Graphical representation of proteins. *Chemical Reviews*, **2011**, 111, 790-862	68.1	88
195	A novel 2-D graphical representation of DNA sequences of low degeneracy. *Chemical Physics Letters* , **2001**, 350, 106-112	2.5	88
194	Random walks and their diagnostic value for characterization of atomic environment. *Journal of Computational Chemistry*, **1980**, 1, 386-399	3.5	87
193	Novel 2-D graphical representation of proteins. *Chemical Physics Letters*, **2006**, 419, 528-532	2.5	86
192	On interpretation of well-known topological indices. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 550-60		85
191	Condensed representation of DNA primary sequences. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 50-6		84
190	Unique graphical representation of protein sequences based on nucleotide triplet codons. *Chemical Physics Letters*, **2004**, 397, 247-252	2.5	83
189	Graphical representations of DNA as 2-D map. *Chemical Physics Letters*, **2004**, 386, 468-471	2.5	79
188	On representation of proteins by star-like graphs. *Journal of Molecular Graphics and Modelling*, **2007** , 26, 290-305	2.8	78
187	Novel shape descriptors for molecular graphs. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 607-13		73
186	Enumeration of the Kekul structures in conjugated hydrocarbons. *Journal of the Chemical Society, Faraday Transactions 2*, **1976**, 72, 232-243		68
185	Conjugation and aromaticity of corannulenes. *Journal of the American Chemical Society*, **1984**, 106, 4428-4434	14.4	67
184	Resonance energy of very large benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, **1980**, 17, 549-586	2.1	66

183	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
182	Optimal Molecular Descriptors Based on Weighted Path Numbers. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 261-266		62
181	Molecular Shape Profiles. *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 373-382		61
180	Compact 2-D graphical representation of DNA. *Chemical Physics Letters*, **2003**, 373, 558-562	2.5	60
179	On a graph theoretical basis for ordering of structures. *Chemical Physics Letters*, **1979**, 63, 332-336	2.5	58
178	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
177	On characterization of DNA primary sequences by a condensed matrix. *Chemical Physics Letters*, **2000**, 317, 29-34	2.5	54
176	On Canonical Numbering of Atoms in a Molecule and Graph Isomorphism. *Journal of Chemical Information and Modeling*, **1977**, 17, 171-180	6.1	54
175	A correlation between Kekul□valence structures and conjugated circuits. *Chemical Physics*, **1979**, 41, 265-270	2.3	51
174	On 3-D graphical representation of proteomics maps and their numerical characterization. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1339-44		50
173	Use of the Szeged index and the revised Szeged index for measuring network bipartivity. *Discrete Applied Mathematics*, **2010**, 158, 1936-1944	1	49
172	PARTITIONING OF □ELECTRONS IN RINGS OF POLYCYCLIC conjugated HYDROCARBONS. PART 1: CATACONDENSED BENZENOIDS. *Polycyclic Aromatic Compounds*, **2004**, 24, 173-193	1.3	49
171	Hierarchical orthogonalization of descriptors. *International Journal of Quantum Chemistry*, **1997**, 63, 215-222	2.1	48
170	Algebraic Kekul□formulas for benzenoid hydrocarbons. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 365-72		48
169	Variable connectivity index for cycle-containing structures. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 657-62		48
168	On a characterization of the folding of proteins. *International Journal of Quantum Chemistry*, **1999**, 75, 1017-1026	2.1	48
167	In search of structural invariants. *Journal of Mathematical Chemistry*, **1992**, 9, 97-146	2.1	48
166	Partitioning of □electrons in rings of polycyclic conjugated hydrocarbons. Part 3. Perifusenes. *New Journal of Chemistry*, **2004**, 28, 800-806	3.6	47

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	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
163	The variable molecular descriptors based on distance related matrices. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 575-81		45
162	Characterization of 3-D sequences of proteins. *Chemical Physics Letters*, **1997**, 272, 115-119	2.5	43
161	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
160	On evaluation of the characteristic polynomial for large molecules. *Journal of Computational Chemistry*, **1982**, 3, 421-435	3.5	43
159	Fitting of nonlinear regressions by orthogonalized power series. *Journal of Computational Chemistry*, **1993**, 14, 363-370	3.5	42
158	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
157	Four-color map representation of DNA or RNA sequences and their numerical characterization. *Chemical Physics Letters*, **2005**, 407, 205-208	2.5	41
156	On characterization of three-dimensional structures. *International Journal of Quantum Chemistry*, **1988**, 34, 201-208	2.1	41
155	Nonempirical approach to structure□ctivity studies. *International Journal of Quantum Chemistry*, **1984**, 26, 137-153	2.1	41
154	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
153	Graph theoretical approach to □electron currents in polycyclic conjugated hydrocarbons. *Chemical Physics Letters*, **2010**, 500, 123-127	2.5	39
152	On characterization of physical properties of amino acids. *International Journal of Quantum Chemistry*, **2000**, 80, 1199-1209	2.1	39
151	On graphical and numerical characterization of proteomics maps. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1330-8		39
150	Symmetry properties of graphs of interest in chemistry. II. Desargues□evi graph. *International Journal of Quantum Chemistry*, **1979**, 15, 663-682	2.1	39
149	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
148	On the evaluation of the characteristic polynomial via symmetric function theory. *Journal of Mathematical Chemistry*, **1987**, 1, 145-152	2.1	38

147	On Unique Numbering of Atoms and Unique Codes for Molecular Graphs. *Journal of Chemical Information and Modeling*, **1975**, 15, 105-108	6.1	38
146	Novel map descriptors for characterization of toxic effects in proteomics maps. *Journal of Molecular Graphics and Modelling*, **2003**, 22, 1-9	2.8	37
145	Optimal molecular connectivity descriptors for nitrogen-containing molecules. *International Journal of Quantum Chemistry*, **1998**, 70, 1209-1215	2.1	36
144	Algorithm for coding DNA sequences into "spectrum-like" and "zigzag" representations. *Journal of Chemical Information and Modeling*, **2005**, 45, 309-13	6.1	36
143	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
142	Characterization of DNA primary sequences based on the average distances between bases. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 561-8		36
141	The conjugated-circuit model: application to benzenoid hydrocarbons. *Journal of Molecular Structure*, **1989**, 198, 223-237	3.4	36
140	On some solved and unsolved problems of chemical graph theory. *International Journal of Quantum Chemistry*, **1986**, 30, 699-742	2.1	35
139	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
138	On structural interpretation of several distance related topological indices. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 593-601		32
137	On Characterization of Cyclic Structures. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 1063-1071		31
136	Algebraic Kekul□structures of benzenoid hydrocarbons. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 296-9		31
135	A new descriptor for structure-property and structure-activity correlations. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 650-6		31
134	Molecular bonding profiles. *Journal of Mathematical Chemistry*, **1996**, 19, 375-392	2.1	31
133	Partitioning of □electrons in Rings of Polycyclic Conjugated Hydrocarbons. Part 4. Benzenoids with More Than One Geometric Kekul□Structure Corresponding to the Same Algebraic Kekul□ Structure. *Journal of Mathematical Chemistry*, **2004**, 36, 271-279	2.1	30
132	Resonance in catacondensed benzenoid hydrocarbons. *International Journal of Quantum Chemistry*, **1997**, 63, 585-600	2.1	29
131	Another look at the chaos-game representation of DNA. *Chemical Physics Letters*, **2008**, 456, 84-88	2.5	29
130	Order from chaos: observing hormesis at the proteome level. *Journal of Proteome Research*, **2005**, 4, 2133-6	5.6	29

129	A graph theoretical characterization of proteomics maps. *International Journal of Quantum Chemistry*, **2002**, 90, 848-858	2.1	29
128	Graph-theoretical analysis of molecular properties. Isomeric variations in nonanes. *International Journal of Quantum Chemistry*, **1980**, 18, 1005-1027	2.1	29
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124	Solved and Unsolved Problems of Structural Chemistry		28
123	Milestones in graphical bioinformatics. *International Journal of Quantum Chemistry*, **2013**, 113, 2413-2446	2.1	26
122	On characterization of dose variations of 2-D proteomics maps by matrix invariants. *Journal of Proteome Research*, **2002**, 1, 217-26	5.6	26
121	On Characterization of Molecular Shapes. *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 594-606		26
120	Symmetry properties of chemical graphs. IX. The valence tautomerism in the P73 skeleton. *Journal of Computational Chemistry*, **1986**, 7, 35-54	3.5	26
119	On Kekulé structures of buckminsterfullerene. *Chemical Physics Letters*, **2005**, 401, 446-450	2.5	25
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115	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
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113	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
112	The anti-adjacency matrix of a graph: Eccentricity matrix. *Discrete Applied Mathematics*, **2018**, 251, 299-309	1	20

111	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
110	Partitioning of π-Electrons in Rings of Fibonacenes. *Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences*, **2005**, 60, 171-176	1.4	20
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107	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
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105	On irreducible endospectral graphs. *Journal of Mathematical Physics*, **1986**, 27, 2601-2612	1.2	18
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100	On a geometry-based approach to protein sequence alignment. *Journal of Mathematical Chemistry*, **2008**, 43, 756-772	2.1	17
99	Composition as a method for data reduction: application to carbon-13 NMR chemical shifts. *Theoretica Chimica Acta*, **1988**, 73, 233-246		17
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93	Novel characterization of proteomics maps by sequential neighborhoods of protein spots. *Journal of Chemical Information and Modeling*, **2005**, 45, 1205-13	6.1	15
92	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
91	Higher-order Fibonacci numbers. *Journal of Mathematical Chemistry*, **1996**, 20, 79-94	2.1	15
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89	A rational selection of graph-theoretical indices in the QSAR. *International Journal of Quantum Chemistry*, **1988**, 34, 267-285	2.1	15
88	Symmetry properties of chemical graphs. IV. Rearrangement of tetragonal-pyramidal complexes. *International Journal of Quantum Chemistry*, **1982**, 21, 647-663	2.1	15
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84	Local aromaticity and aromatic sextet theory beyond Clar. *International Journal of Quantum Chemistry*, **2018**, 118, e25657	2.1	13
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82	Restricted random walks on graphs. *Theoretica Chimica Acta*, **1995**, 92, 97-106		13
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80	Symmetry properties of chemical graphs. VI. Isomerizations of octahedral complexes. *International Journal of Quantum Chemistry*, **1984**, 26, 69-89	2.1	13
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66	Very efficient search for nucleotide alignments. *Journal of Computational Chemistry*, **2013**, 34, 77-82	3.5	10
65	Correlations between various ways of accounting for the distribution of π-electrons in benzenoids. *New Journal of Chemistry*, **2008**, 32, 1071	3.6	10
64	A graph theoretical approach to Möbius systems in organic chemistry. *International Journal of Quantum Chemistry*, **1986**, 30, 185-201	2.1	10
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61	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
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32	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
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