Ramon CarbÃ³-Dorca i CarrÃ©

List of Publications by Year
in descending order

293 papers	8,238 citations	53751 45 h-index	74108 75 g-index
300 all docs	300 docs citations	300 times ranked	2945 citing authors

#	Article	IF	Citations
1	How similar is a molecule to another? An electron density measure of similarity between two molecular structures. International Journal of Quantum Chemistry, 1980, 17, 1185-1189.	1.0	640
2	Critical analysis and extension of the Hirshfeld atoms in molecules. Journal of Chemical Physics, 2007, 126, 144111.	1.2	577
3	Electron Delocalization and Aromaticity in Linear Polyacenes:â€‰ Atoms in Molecules Multicenter Delocalization Index. Journal of Physical Chemistry A, 2006, 110, 7642-7648.	1.1	176
4	Critical thoughts on computing atom condensed Fukui functions. Journal of Chemical Physics, 2007, 127, 034102.	1.2	162
5	Molecular quantum similarity measures andN-dimensional representation of quantum objects. I. Theoretical foundations. International Journal of Quantum Chemistry, 1992, 42, 1681-1693.	1.0	126
6	Quantum similarity measures under atomic shell approximation: First order density fitting using elementary Jacobi rotations. Journal of Computational Chemistry, 1997, 18, 2023-2039.	1.5	117
7	Negative Fukui functions: New insights based on electronegativity equalization. Journal of Chemical Physics, 2003, 118, 4349-4356.	1.2	114
8	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
9	A general survey of molecular quantum similarity. Computational and Theoretical Chemistry, 1998, 451, 11-23.	1.5	108
10	Toward a global maximization of the molecular similarity function: Superposition of two molecules. Journal of Computational Chemistry, 1997, 18, 826-846.	1.5	100
11	Molecular Quantum Similarity and the Fundamentals of QSAR. Accounts of Chemical Research, 2002, 35, 289-295.	7.6	99
12	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	1.1	99
13	Atomic Shell Approximation: Electron Density Fitting Algorithm Restricting Coefficients to Positive Values. Journal of Chemical Information and Computer Sciences, 1995, 35, 1046-1053.	2.8	95
14	Three-Dimensional Quantitative Structureâ^'Activity Relationships from Tuned Molecular Quantum Similarity Measures:â€‰ Prediction of the Corticosteroid-Binding Globulin Binding Affinity for a Steroid Family. Journal of Chemical Information and Computer Sciences, 1999, 39, 333-344.	2.8	91
15	Molecular Quantum Similarity: theoretical Framework, Ordering Principles, and Visualization Techniques. Advances in Quantum Chemistry, 1994, , 253-313.	0.4	89
16	Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284.	1.5	76
17	Quantum molecular similarity measures (QMSM) as a natural way leading towards a theoretical foundation of quantitative structure-properties relationships (QSPR). Journal of Mathematical Chemistry, 1995, 18, 237-246.	0.7	75
18	Fitted electronic density functions from H to Rn for use in quantum similarity measures: cis-diamminedichloroplatinum(II) complex as an application example. Journal of Computational Chemistry, 1999, 20, 911-920.	1.5	75

#	Article	IF	Citations
19	Quantum Mechanical Basis for Mulliken Population Analysis. Journal of Mathematical Chemistry, 2004, 36, 231-239.	0.7	74
20	TGSA: A molecular superposition program based on topo-geometrical considerations. Journal of Computational Chemistry, 2001, 22, 255-263.	1.5	70
21	Molecular quantum similarity measures andN-dimensional representation of quantum objects. II. Practical applications. International Journal of Quantum Chemistry, 1992, 42, 1695-1709.	1.0	69
22	Quantum mechanical origin of QSAR: theory and applications. Computational and Theoretical Chemistry, 2000, 504, 181-228.	1.5	69
23	Molsimil - 88: Molecular similarity calculations using a CNDO-like approximation. Computer Physics Communications, 1989, 55, 117-126.	3.0	67
24	Molecular basis of quantitative structure-properties relationships (QSPR): a quantum similarity approach. Journal of Computer-Aided Molecular Design, 1999, 13, 259-270.	1.3	64
25	Structure-Activity Relationships of a Steroid Family using Quantum Similarity Measures and Topological Quantum Similarity Indices. QSAR and Combinatorial Science, 1997, 16, 465-472.	1.4	62
26	A Mathematical Discussion on Density and Shape Functions, Vector Semispaces and Related Questions. Journal of Mathematical Chemistry, 2004, 36, 191-200.	0.7	61
27	Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. Structural Chemistry, 2018, 29, 33-38.	1.0	61
28	On quantum molecular similarity measures (QMSM) and indices (QMSI). Journal of Mathematical Chemistry, 1996, 19, 47-56.	0.7	59
29	Inward matrix products: extensions and applications to quantum mechanical foundations of QSAR. Computational and Theoretical Chemistry, 2001, 537, 41-54.	1.5	59
30	Quantum similarity measures, molecular cloud description, and structure-properties relationships. Journal of Chemical Information and Computer Sciences, 1992, 32, 600-606.	2.8	58
31	Application of Molecular Quantum Similarity to QSAR. QSAR and Combinatorial Science, 1997, 16, 25-32.	1.4	58
32	Molecular Quantum Similarity Measures Tuned 3D QSAR:â€‰ An Antitumoral Family Validation Study. Journal of Chemical Information and Computer Sciences, 1998, 38, 624-631.	2.8	57
33	Negative and Infinite Fukui Functions: The Role of Diagonal Dominance in the Hardness Matrix. Journal of Mathematical Chemistry, 2003, 34, 67-74.	0.7	56
34	Molecular Electronic Density Fitting Using Elementary Jacobi Rotations under Atomic Shell Approximation. Journal of Chemical Information and Computer Sciences, 2000, 40, 1188-1198.	2.8	55
35	Use of ab Initio Quantum Molecular Similarities as an Interpretative Tool for the Study of Chemical Reactions. Journal of the American Chemical Society, 1994, 116, 5909-5915.	6.6	54
36	A comparative analysis by means of quantum molecular similarity measures of density distributions derived from conventional ab initio and density functional methods. Journal of Chemical Physics, 1996, 104, 636-647.	1.2	54

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37	Definition and quantum chemical applications of nested summation symbols and logical functions: Pedagogical artificial intelligence devices for formulae writing, sequential programming and automatic parallel implementation. Journal of Mathematical Chemistry, 1995, 18, 37-72.	0.7	53
38	Molecular quantum similarity measures as an alternative to log P values in QSAR studies. Journal of Computational Chemistry, 1998, 19, 1575-1583.	1.5	53
39	The Fukui matrix: a simple approach to the analysis of the Fukui function and its positive character. Physical Chemistry Chemical Physics, 2011, 13, 6110.	1.3	53
40	Foundation of quantum similarity measures and their relationship to QSPR: Density function structure, approximations, and application examples. International Journal of Quantum Chemistry, 2005, 101, 8-20.	1.0	51
41	Aromaticity in linear polyacenes: Generalized population analysis and molecular quantum similarity approach. Journal of Computational Chemistry, 2007, 28, 152-160.	1.5	51
42	Triple density molecular quantum similarity measures: A general connection between theoretical calculations and experimental results. Molecular Engineering, 1992, 2, 43-64.	0.2	48
43	Communications on quantum similarity, part 3: A geometricâ€quantum similarity molecular superposition algorithm. Journal of Computational Chemistry, 2011, 32, 582-599.	1.5	48
44	On the calculation ofab initioquantum molecular similarities for large systems: Fitting the electron density. Journal of Computational Chemistry, 1994, 15, 1113-1120.	1.5	46
45	Modeling Antimalarial Activity:â€‰ Application of Kinetic Energy Density Quantum Similarity Measures as Descriptors in QSAR. Journal of Chemical Information and Computer Sciences, 2000, 40, 1400-1407.	2.8	46
46	Use of promolecular ASA density functions as a general algorithm to obtain starting MO in SCF calculations. International Journal of Quantum Chemistry, 2002, 87, 59-67.	1.0	46
47	Quantum similarity approach to LFER: substituent and solvent effects on the acidities of carboxylic acids. Journal of Physical Organic Chemistry, 1999, 12, 447-454.	0.9	45
48	Title is missing!. Journal of Mathematical Chemistry, 2002, 32, 201-223.	0.7	45
49	Molecular Quantum Similarity Analysis of Estrogenic Activity. Journal of Chemical Information and Computer Sciences, 2003, 43, 1166-1176.	2.8	45
50	Definition, mathematical examples and quantum chemical applications of nested summation symbols and logical Kronecker deltas. Computers & Chemistry, 1994, 18, 117-126.	1.2	44
51	Simple Linear QSAR Models Based on Quantum Similarity Measures. Journal of Medicinal Chemistry, 1999, 42, 5169-5180.	2.9	44
52	Quantum Similarity Superposition Algorithm (QSSA):â€‰ A Consistent Scheme for Molecular Alignment and Molecular Similarity Based on Quantum Chemistry. Journal of Chemical Information and Computer Sciences, 2003, 43, 1143-1150.	2.8	44
53	Fuzzy sets and boolean tagged sets; vector semispaces and convex sets; quantum similarity measures and asa density functions; diagonal vector spaces and quantum chemistry. Advances in Molecular Similarity, 1999, , 43-72.	0.5	43
54	Tagged sets, convex sets and quantum similarity measures. Journal of Mathematical Chemistry, 1998, 23, 353-364.	0.7	42

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55	Commentaries on quantum similarity (1): Density gradient quantum similarity. Journal of Computational Chemistry, 2010, 31, 2195-2212.	1.5	42
56	Fuzzy sets and Boolean tagged sets. Journal of Mathematical Chemistry, 1997, 22, 143-147.	0.7	40
57	Identification of Active Molecular Sites Using Quantum-Self-Similarity Measures. Journal of Chemical Information and Computer Sciences, 2001, 41, 978-991.	2.8	39
58	Chemical structures from the analysis of domain-averaged Fermi holes: Multiple metalï£¿metal bonding in transition metal compounds. Journal of Computational Chemistry, 2003, 24, 1829-1838.	1.5	39
59	Shells, point cloud huts, generalized scalar products, cosines and similarity tensor representations in vector semispaces. Journal of Mathematical Chemistry, 2012, 50, 210-219.	0.7	39
60	Modelling Toxicity using Molecular Quantum Similarity Measures. QSAR and Combinatorial Science, 2006, 25, 579-589.	1.5	38
61	Structure-activity relations of phenethylamine. Comparison of quantum mechanical SCF ab initio and semiempirical calculations. Journal of the American Chemical Society, 1975, 97, 1338-1347.	6.6	36
62	A Formal Comparison between Molecular Quantum Similarity Measures and Indices. Journal of Chemical Information and Computer Sciences, 1998, 38, 469-475.	2.8	36
63	Use of electron-electron repulsion energy as a molecular descriptor in QSAR and QSPR studies. Journal of Computer-Aided Molecular Design, 2000, 14, 477-485.	1.3	36
64	Quality of Approximate Electron Densities and Internal Consistency of Molecular Alignment Algorithms in Molecular Quantum Similarity. Journal of Chemical Information and Computer Sciences, 2003, 43, 1208-1217.	2.8	36
65	Maximal probability domains in linear molecules. Journal of Computational Chemistry, 2005, 26, 455-460.	1.5	36
66	Some remarks about a generalized SCF coupling operator open shell theory. Chemical Physics Letters, 1975, 30, 43-48.	1.2	34
67	Aromatic Compounds Aquatic Toxicity QSAR Using Molecular Quantum Similarity Measures. SAR and QSAR in Environmental Research, 1999, 10, 401-422.	1.0	34
68	Stochastic transformation of quantum similarity matrices and their use in quantum QSAR (QQSAR) models. International Journal of Quantum Chemistry, 2000, 79, 163-177.	1.0	34
69	Elementary Unitary MO Transformations and SCF Theory. Advances in Quantum Chemistry, 1982, 15, 215-265.	0.4	33
70	Nested summation symbols and perturbation theory. Journal of Mathematical Chemistry, 1993, 13, 331-342.	0.7	33
71	Quantum molecular similarity measures and the n-dimensional representation of a molecular set: phenyldimethylthiazines. Computational and Theoretical Chemistry, 1992, 254, 517-531.	1.5	32
72	Structure-toxicity relationships of polycyclic aromatic hydrocarbons using molecular quantum similarity. Journal of Computer-Aided Molecular Design, 2001, 15, 67-80.	1.3	32

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73	Notes on quantitative structureâ€properties relationships (QSPR) (1): A discussion on a QSPR dimensionality paradox (QSPR DP) and its quantum resolution. Journal of Computational Chemistry, 2009, 30, 1146-1159.	1.5	32
74	A comparative study of isodensity surfaces using ab initio and ASA density functions. Journal of Molecular Graphics and Modelling, 1998, 16, 190-196.	1.3	31
75	Title is missing!. Journal of Mathematical Chemistry, 2001, 30, 227-245.	0.7	31
76	Natural Vector Spaces (inward power and Minkowski norm of a Natural Vector, Natural Boolean) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 6 914-940.	0.7	31
77	General trends in atomic and nuclear quantum similarity measures. International Journal of Quantum Chemistry, 2000, 77, 685-692.	1.0	30
78	Molecular Quantum Similarity Matrix Based Clustering of Molecules Using Dendrograms. Journal of Chemical Information and Computer Sciences, 2003, 43, 170-177.	2.8	30
79	A General Procedure to Obtain Quantum Mechanical Charge and Bond Order Molecular Parameters. Journal of Mathematical Chemistry, 2004, 36, 201-210.	0.7	30
80	Coulomb and Overlap Self-Similarities:Â A Comparative Selectivity Analysis of Structureâ˜Function Relationships for Auxinâ˜like Molecules. Journal of Chemical Information and Modeling, 2006, 46, 1751-1762.	2.5	30
81	Quantum Molecular Similarity: Theory and Applications to the Evaluation of Molecular Properties, Biological Activities and Toxicity. Mathematical and Computational Chemistry, 2001, , 187-320.	0.3	30
82	Fast Calculation of Quantum Chemical Molecular Descriptors from the Electronegativity Equalization Method. Journal of Chemical Information and Computer Sciences, 2003, 43, 422-428.	2.8	29
83	Molecular quantum similarity using conceptual DFT descriptors. Journal of Chemical Sciences, 2005, 117, 425-435.	0.7	29
84	Analyzing the Triple Density Molecular Quantum Similarity Measures with the INDSCAL Model. Journal of Chemical Information and Computer Sciences, 1998, 38, 620-623.	2.8	27
85	Application of promolecular asa densities to graphical representation of density functions of macromolecular systems. Journal of Molecular Graphics and Modelling, 2001, 19, 343-348.	1.3	27
86	Molecular Basis of LFER. Modeling of the Electronic Substituent Effect Using Fragment Quantum Self-Similarity Measures. Journal of Chemical Information and Computer Sciences, 2003, 43, 2033-2038.	2.8	27
87	About the prediction of molecular properties using the fundamental Quantum QSPR (QQSPR) equationâ€. SAR and QSAR in Environmental Research, 2007, 18, 265-284.	1.0	27
88	Molecular quantum similarity measures in Minkowski metric vector semispaces. Journal of Mathematical Chemistry, 2008, 44, 628-636.	0.7	27
89	Communications on quantum similarity (4): collective distances computed by means of similarity matrices, as generators of intrinsic ordering among quantum multimolecular polyhedra. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 380-404.	6.2	27
90	Quantum polyhedra, definitions, statistics and the construction of a collective quantum similarity index. Journal of Mathematical Chemistry, 2015, 53, 171-182.	0.7	27

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91	Unconditional convergence in SCF theory: a general level shift technique. Chemical Physics Letters, 1977, 47, 581-583.	1.2	26
92	Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. Computational and Theoretical Chemistry, 1996, 371, 171-183.	1.5	26
93	Title is missing!. Journal of Mathematical Chemistry, 1998, 23, 365-375.	0.7	26
94	Using Molecular Quantum Similarity Measures as Descriptors in Quantitative Structure-Toxicity Relationships. SAR and QSAR in Environmental Research, 1999, 10, 545-556.	1.0	26
95	Modeling Large Macromolecular Structures Using Promolecular Densities. Journal of Chemical Information and Computer Sciences, 2002, 42, 847-852.	2.8	26
96	Estimation of infinite dilution activity coefficients of organic compounds in water with neural classifiers. AICHE Journal, 2004, 50, 1315-1343.	1.8	26
97	Notes on quantitative structureâ€“property relationships (QSPR), part 3: Density functions origin shift as a source of quantum QSPR algorithms in molecular spaces. Journal of Computational Chemistry, 2013, 34, 766-779.	1.5	26
98	N-dimensional Boolean hypercubes and the goldbach conjecture. Journal of Mathematical Chemistry, 2016, 54, 1213-1220.	0.7	26
99	Quantum molecular similarity measures. Advances in Molecular Similarity, 1996, , 1-42.	0.5	26
100	Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M) Tj ETQq0 0 0 rgBT /Overlock 10 T 1047-1053.	2.8	25
101	Quantification of the Influence of Single-Point Mutations on Haloalkane Dehalogenase Activity:â€‰ A Molecular Quantum Similarity Study. Journal of Chemical Information and Computer Sciences, 2000, 40, 839-846.	2.8	25
102	Quantum similarity and discrete representation of molecular sets. Journal of Mathematical Chemistry, 2011, 49, 1558-1572.	0.7	25
103	Centroid origin shift of quantum object sets and molecular point clouds description and element comparisons. Journal of Mathematical Chemistry, 2012, 50, 1161-1178.	0.7	25
104	Quantum molecular similarity measures (QMSM) and the atomic shell approximation (ASA). Advances in Molecular Similarity, 1996, , 187-211.	0.5	25
105	Solutions to the Quantum QSPR problem in molecular spaces. Theoretical Chemistry Accounts, 2007, 118, 673-679.	0.5	24
106	Quantum Similarity and Quantum Quantitative Structure-Properties Relationships (QQSPR). , 2009, , 7422-7480.		24
107	Fundamental quantum QSAR (Q2SAR) equation: extensions, nonlinear terms, and generalizations within extended Hilbert-Sobolev spaces. International Journal of Quantum Chemistry, 2002, 88, 167-182.	1.0	23
108	TGSA-Flex: Extending the capabilities of the Topo-Geometrical superposition algorithm to handle flexible molecules. Journal of Computational Chemistry, 2004, 25, 153-159.	1.5	23

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109	Select-divide-and-conquer method for large-scale configuration interaction. Journal of Chemical Physics, 2006, 125, 014108.	1.2	23
110	Construction of coherent nano quantitative structureâ€“properties relationships (nano-QSPR) models and catastrophe theory. SAR and QSAR in Environmental Research, 2011, 22, 661-665.	1.0	23
111	Many Center AO Integral Evaluation Using Cartesian Exponential Type Orbitals (CETO'S). Advances in Quantum Chemistry, 1992, , 115-237.	0.4	21
112	On the extension of quantum similarity to atomic nuclei: Nuclear quantum similarity. Journal of Mathematical Chemistry, 1998, 23, 327-351.	0.7	21
113	Inward matrix products, generalised density functions and Rayleighâ€“SchrÃ¶dinger perturbation theory. Computational and Theoretical Chemistry, 2000, 501-502, 173-176.	1.5	21
114	Molecular Basis of Linear Free Energy Relationships. The Nature of Inductive Effect in Aliphatic Series. Journal of Chemical Information and Computer Sciences, 2002, 42, 564-570.	2.8	21
115	A new insight on the quantum quantitative structureâ€properties relationships. International Journal of Quantum Chemistry, 2008, 108, 1721-1734.	1.0	21
116	Multimolecular polyhedra and QSPR. Journal of Mathematical Chemistry, 2014, 52, 1848-1856.	0.7	21
117	DNA, unnatural base pairs and hypercubes. Journal of Mathematical Chemistry, 2018, 56, 1353-1356.	0.7	21
118	Divagations about the periodic table: Boolean hypercube and quantum similarity connections. Journal of Computational Chemistry, 2019, 40, 2653-2663.	1.5	21
119	Rational modelling of the voltage-dependent K+ channel inactivation by aminopyridines. Biophysical Chemistry, 2003, 104, 417-427.	1.5	20
120	Structureâ€”property relationships and momentum space quantities: Hammett Ïƒâ€”constants. Molecular Physics, 2003, 101, 3159-3162.	0.8	20
121	Unrevealed structural requirements for auxin-like molecules by theoretical and experimental evidences. Phytochemistry, 2007, 68, 237-250.	1.4	20
122	Collective Euclidian distances and quantum similarity. Journal of Mathematical Chemistry, 2013, 51, 338-353.	0.7	20
123	Extended density functions. Advances in Quantum Chemistry, 2000, 38, 1-63.	0.4	19
124	Algebraic relationships between conceptual DFT quantities and the electronegativity equalization hardness matrix. Chemical Physics Letters, 2002, 364, 357-362.	1.2	19
125	Similarity approach to QSAR. International Journal of Pharmaceutics, 2004, 269, 51-60.	2.6	19
126	Definition of norm coherent generalized scalar products and quantum similarity. Journal of Mathematical Chemistry, 2010, 47, 331-344.	0.7	19

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127	Open Shell SCF Theory: An ab Initio Study of Some Interstellar Molecules. Advances in Quantum Chemistry, 1980, 12, 159-187.	0.4	18
128	Facet diagrams for quantum similarity data. Journal of Computer-Aided Molecular Design, 1999, 13, 597-610.	1.3	18
129	Quantum similarity QSAR: Study of inhibitors binding to thrombin, trypsin, and factor Xa, including a comparison with CoMFA and CoMSIA methods. International Journal of Quantum Chemistry, 2000, 80, 265-282.	1.0	18
130	Antimalarial activity of synthetic 1,2,4-trioxanes and cyclic peroxy ketals, a quantum similarity study. Journal of Computer-Aided Molecular Design, 2001, 15, 1053-1063.	1.3	18
131	Non-linear Terms & Variational Approach in Quantum QSPR. Journal of Mathematical Chemistry, 2004, 36, 241-260.	0.7	18
132	Communications on quantum similarity (2): A geometric discussion on holographic electron density theorem and confined quantum similarity measures. Journal of Computational Chemistry, 2010, 31, 2452-2462.	1.5	18
133	Mathematical aspects of the LCAO MO first order density function (5): centroid shifting of MO shape functions basis set, properties and applications. Journal of Mathematical Chemistry, 2013, 51, 289-296.	0.7	18
134	About ErdÃ¶s discrepancy conjecture. Journal of Mathematical Chemistry, 2016, 54, 657-660.	0.7	18
135	All valence electron wavefunctions and electrostatic molecular potentials under zero differential overlap approximation. Chemical Physics Letters, 1974, 25, 89-91.	1.2	17
136	Empirical quantum chemical approach to structure-gas chromatographic retention index relationships. Journal of Chromatography A, 1975, 108, 337-344.	1.8	17
137	Quantum QSAR and the eigensystems of stochastic quantum similarity matrices. Journal of Mathematical Chemistry, 2000, 27, 357-376.	0.7	17
138	Applications of inward matrix products and matrix wave functions to HÃ¼ckel MO theory, Slater extended wave functions, spin extended functions, and Hartree method. International Journal of Quantum Chemistry, 2003, 91, 607-617.	1.0	17
139	Scaled Euclidian distances: a general dissimilarity index with a suitably defined geometrical foundation. Journal of Mathematical Chemistry, 2012, 50, 734-740.	0.7	17
140	An isometric representation problem in quantum multimolecular polyhedra and similarity. Journal of Mathematical Chemistry, 2015, 53, 1750-1758.	0.7	17
141	A general multiconfiguration paired excitation self-consistent field theory (MC PE SCF). Chemical Physics Letters, 1977, 47, 85-91.	1.2	16
142	Molecular Quantum Similarity-Based QSARs for Binding Affinities of Several Steroid Sets. Journal of Chemical Information and Computer Sciences, 2002, 42, 1185-1193.	2.8	16
143	Toward an Alternative Hardness Kernel Matrix Structure in the Electronegativity Equalization Method (EEM). Journal of Chemical Information and Modeling, 2006, 46, 1657-1665.	2.5	16
144	A quantum similarity matrix (QSM) Aufbau procedure. Journal of Mathematical Chemistry, 2008, 44, 228-234.	0.7	16

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145	Quantum similarity matrices column set as holograms of DF molecular point clouds. Journal of Mathematical Chemistry, 2012, 50, 2339-2341.	0.7	16
146	Quantum similarity. Advances in Molecular Similarity, 1999, , 1-42.	0.5	16
147	Mathematical Elements of Quantum Electronic Density Functions. Advances in Quantum Chemistry, 2005, , 121-207.	0.4	15
148	Notes on quantitative structureâ€properties relationships (QSPR) part 2: The role of the number of atoms as a molecular descriptor. Journal of Computational Chemistry, 2009, 30, 2099-2104.	1.5	15
149	A Gaussian holographic theorem and the projection of electronic density functions into the surface of a sphere. Journal of Mathematical Chemistry, 2010, 48, 914-924.	0.7	15
150	The general Gaussian product theorem. Journal of Mathematical Chemistry, 2011, 49, 1769-1784.	0.7	15
151	Toward a universal quantum QSPR operator. International Journal of Quantum Chemistry, 2018, 118, e25602.	1.0	15
152	The perturbation theory for non-degenerate states and the extended Hï¿½ckel method. Theoretica Chimica Acta, 1970, 17, 74-80.	0.9	14
153	Extending molecular similarity to energy surfaces: Boltzmann similarity measures and indices. Journal of Mathematical Chemistry, 1996, 20, 247-261.	0.7	14
154	Quantum similarity, volume functions and generalized CarbÃ³ indices. Journal of Mathematical Chemistry, 2011, 49, 2109-2115.	0.7	14
155	About the concept of Chemical Space: a concerned reflection on some trends of modern scientific thought within theoretical chemical lore. Journal of Mathematical Chemistry, 2013, 51, 413-419.	0.7	14
156	Aromaticity, quantum multimolecular polyhedra, and quantum QSPR fundamental equation. Journal of Computational Chemistry, 2016, 37, 78-82.	1.5	14
157	A study on Goldbach conjecture. Journal of Mathematical Chemistry, 2016, 54, 1798-1809.	0.7	14
158	Boolean Hypercubes as time representation holders. Journal of Mathematical Chemistry, 2018, 56, 1349-1352.	0.7	14
159	Electrostatic molecular potential as a static index in the study of aromatic substitutions. Chemical Physics Letters, 1975, 31, 267-270.	1.2	13
160	Electrostatic corrections to extended HÃ¼ckel theory. International Journal of Quantum Chemistry, 1977, 11, 271-276.	1.0	13
161	A naive look on the Hohenbergâ€“Kohn theorem. Journal of Mathematical Chemistry, 1999, 25, 253-257.	0.7	13
162	Icosahedral symmetry structures with open-shell electronic configuration hN (N=1â€“9).. Physics Letters, Section A: General, Atomic and Solid State Physics, 2000, 267, 370-378.	0.9	13

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163	Smooth function topological structure descriptors based on graph-spectra. Journal of Mathematical Chemistry, 2008, 44, 373-378.	0.7	13
164	Mathematical aspects of the LCAO MO first order density function (4): a discussion on the connection of Taylor series expansion of electronic density (TSED) function with the holographic electron density theorem (HEDT) and the Hohenberg-Kohn theorem (HKT). Journal of Mathematical Chemistry, 2011, 49, 836-842.	0.7	13
165	EMP as a similarity measure: a geometric point of view. Journal of Mathematical Chemistry, 2013, 51, 382-389.	0.7	13
166	Refinement of a generalized Fermatâ€™s last theorem conjecture in natural vector spaces. Journal of Mathematical Chemistry, 2017, 55, 1869-1877.	0.7	13
167	Role of the structure of Boolean hypercubes when used as vectors in natural (Boolean) vector semispaces. Journal of Mathematical Chemistry, 2019, 57, 697-700.	0.7	13
168	Chemical bonds from the condition of minimal pair fluctuation: Correlated case. International Journal of Quantum Chemistry, 1999, 72, 85-91.	1.0	12
169	Title is missing!. Journal of Mathematical Chemistry, 2003, 33, 227-244.	0.7	12
170	Classification of reaction pathways via momentumâ€“space and quantum molecular similarity measures. Chemical Physics Letters, 2003, 367, 207-213.	1.2	12
171	Least squares estimation of unknown molecular properties and quantum QSPR fundamental equation. Journal of Mathematical Chemistry, 2015, 53, 1651-1656.	0.7	12
172	Quantum polyhedra in LCAO MO theory. Molecular Physics, 2016, 114, 1236-1249.	0.8	12
173	Cantor-like transfinite sequences and GÃ¶del-like incompleteness revealed by means of Mersenne transfinite dimensional boolean hypercube concatenation. Journal of Mathematical Chemistry, 2020, 58, 1-5.	0.7	12
174	Boolean hypercubes and the structure of vector spaces. Journal of Mathematical Sciences and Modelling, 2018, 1, 1-14.	0.2	12
175	A concurrent algorithm for parallel calculation of eigenvalues and eigenvectors of real symmetric matrices. Journal of Computational Chemistry, 1992, 13, 155-159.	1.5	11
176	Generalized Rayleigh-Schrï¿½dinger perturbation theory in matrix form. Journal of Mathematical Chemistry, 1994, 15, 397-406.	0.7	11
177	Diagonal coefficient representation of density functions and quantum similarity measures. Journal of Mathematical Chemistry, 2008, 44, 621-627.	0.7	11
178	Hypercubes defined on n-ary sets, the ErdÃ¶sâ€“Faberâ€“LovÃ¡sz conjecture on graph coloring, and the description spaces of polypeptides and RNA. Journal of Mathematical Chemistry, 2019, 57, 2182-2194.	0.7	11
179	Ground and first excited states electrostatic molecular potentials of ketene and diazomethane. Chemical Physics Letters, 1974, 28, 422-426.	1.2	10
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181	Jacobi Rotations: A General Procedure for Electronic Energy Optimization. Advances in Quantum Chemistry, 1989, 20, 375-441.	0.4	10
182	Ariadne-88: An ab initio monoconfigurational closed and open shell direct electronic energy calculation using elementary Jacobi rotations. Computer Physics Communications, 1989, 52, 345-354.	3.0	10
183	Molecular Quantum Similarity Measures as Descriptors for Quantum QSAR. Polycyclic Aromatic Compounds, 2001, 19, 51-71.	1.4	10
184	Using Molecular Quantum Similarity Measures under Stochastic Transformation To Describe Physical Properties of Molecular Systems. Journal of Chemical Information and Computer Sciences, 2002, 42, 317-325.	2.8	10
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