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	The Collatz conjecture and the quantum mechanical harmonic oscillator. Journal of Mathematical Chemistry, 2022, 60, 145-160.	0.7	4
2	Shadowsâ€™ hypercube, vector spaces, and non-linear optimization of QSPR procedures. Journal of Mathematical Chemistry, 2022, 60, 283-310.	0.7	9
3	Determination of unknown molecular properties in molecular spaces. Journal of Mathematical Chemistry, 2022, 60, 353-359.	0.7	6
4	Average energy and quantum similarity of a time dependent quantum system subject to PÃ¶schlâ€“Teller potential. Journal of Mathematical Chemistry, 2022, 60, 1-21.	0.7	3
5	A naÃ¯ve HMO study of the casimir effect. Journal of Mathematical Chemistry, 2022, 60, 581.	0.7	2
6	Analysis of solutions of time-dependent SchrÃ¶dinger equation of a particle trapped in a spherical box. Journal of Mathematical Chemistry, 2022, 60, 1089-1106.	0.7	7
7	Mersenne Numbers, Recursive Generation of Natural Numbers, and Counting the Number of Prime Numbers. Applied Mathematics, 2022, 13, 538-543.	0.1	3
8	Three conjectures on extended twin primes and the existence of isoboolean and singular primes inspired by relativistic quantum computing. Journal of Mathematical Chemistry, 2022, 60, 1571-1583.	0.7	2
9	About the construction of probability hypercubes. Journal of Mathematical Chemistry, 2021, 59, 1151-1154.	0.7	0
10	An HPC hybrid parallel approach to the experimental analysis of Fermatâ€™s theorem extension to arbitrary dimensions on heterogeneous computer systems. Journal of Supercomputing, 2021, 77, 11328-11352.	2.4	6
11	Generalized scalar products in Minkowski metric spaces. Journal of Mathematical Chemistry, 2021, 59, 1029-1045.	0.7	9
12	Enfolding N-dimensional Euclidean spaces with N-dimensional spheres as a framework to define the structure of time foam. Journal of Mathematical Chemistry, 2021, 59, 1450.	0.7	1
13	Molecular spaces and the dimension paradox. Pure and Applied Chemistry, 2021, 93, 1189-1196.	0.9	3
14	Extended Minkowski spaces, zero norms, and Minkowski hypersurfaces. Journal of Mathematical Chemistry, 2021, 59, 1875-1879.	0.7	6
15	Extension of Fermatâ€™s last theorem in Minkowski natural spaces. Journal of Mathematical Chemistry, 2021, 59, 1851-1863.	0.7	4
16	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
17	A quantum similarity discussion about Einsteinâ€“Podolskyâ€“Rosen (EPR) paradox in Gaussian enfolded spaces. Journal of Mathematical Chemistry, 2020, 58, 1815-1827.	0.7	5
18	Fuzzy Hypercubes and their time-like evolution. Journal of Mathematical Chemistry, 2020, 58, 1337-1344.	0.7	7

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19	Boolean Hypercubes, Mersenne Numbers, and the Collatz Conjecture. Journal of Mathematical Sciences and Modelling, 2020, 3, 120-129.	0.2	4
20	Divagations about the periodic table: Boolean hypercube and quantum similarity connections. Journal of Computational Chemistry, 2019, 40, 2653-2663.	1.5	21
21	Nine questions on energy decomposition analysis. Journal of Computational Chemistry, 2019, 40, 2248-2283.	1.5	113
22	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
23	Vector spaces defined over the unit interval. Journal of Mathematical Chemistry, 2019, 57, 691-693.	0.7	0
24	â€œSolved and unsolved problems of structural chemistryâ€• by Milan RandiÄ‡, Marjana NoviÄ, and Dejan PlavÅ¡iÄ‡ CRC Press, Boca Raton, 2016, XX+472 pp. ISBN 13â€‰978â€‰1â€‰4987â€‰1151â€‰7. Journal of Computational Chemistry, 2019, 40, 1880-1880.	n.a.	0
25	Universal transformation and non-linear connection between experimental and calculated property vectors in QSPR. Journal of Mathematical Chemistry, 2019, 57, 1075-1087.	0.7	5
26	Transformation of boolean hypercube vertices into unit interval elements: QSPR workout consequences. Journal of Mathematical Chemistry, 2019, 57, 694-696.	0.7	7
27	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
28	Toward a universal quantum QSPR operator. International Journal of Quantum Chemistry, 2018, 118, e25602.	1.0	15
29	Boolean Hypercubes as time representation holders. Journal of Mathematical Chemistry, 2018, 56, 1349-1352.	0.7	14
30	DNA, unnatural base pairs and hypercubes. Journal of Mathematical Chemistry, 2018, 56, 1353-1356.	0.7	21
31	Thermal scaling of electronic energy expressions. Journal of Mathematical Chemistry, 2018, 56, 979-981.	0.7	0
32	Atomic thermal voltage population distributions. Journal of Mathematical Chemistry, 2018, 56, 1357-1359.	0.7	0
33	Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. Structural Chemistry, 2018, 29, 33-38.	1.0	61
34	Statistical-like signature of molecular basis sets. Journal of Molecular Modeling, 2018, 24, 256.	0.8	2
35	Boolean hypercubes and the structure of vector spaces. Journal of Mathematical Sciences and Modelling, 2018, 1, 1-14.	0.2	12
36	A theorem on the Gram matrix of a polyhedron. Journal of Mathematical Chemistry, 2017, 55, 79-97.	0.7	6

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37	Refinement of a generalized Fermatâ€™s last theorem conjecture in natural vector spaces. Journal of Mathematical Chemistry, 2017, 55, 1869-1877.	0.7	13
38	Natural Vector Spaces (inward power and Minkowski norm of a Natural Vector, Natural Boolean) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 7 914-940.	0.7	31
39	Aromaticity, quantum multimolecular polyhedra, and quantum QSPR fundamental equation. Journal of Computational Chemistry, 2016, 37, 78-82.	1.5	14
40	On the nature of the collective quantum mechanical description of molecular atoms and bonds. Journal of Mathematical Chemistry, 2016, 54, 1440-1446.	0.7	4
41	N-dimensional Boolean hypercubes and the goldbach conjecture. Journal of Mathematical Chemistry, 2016, 54, 1213-1220.	0.7	26
42	Time vectors and particle swarms defined as polyhedra in spherically enfolded spaces. Journal of Mathematical Chemistry, 2016, 54, 1751-1757.	0.7	9
43	A study on Goldbach conjecture. Journal of Mathematical Chemistry, 2016, 54, 1798-1809.	0.7	14
44	About an incoherent precision behavior in LCAO MO theory when a simple diatomic molecule collapses into an atom. Journal of Mathematical Chemistry, 2016, 54, 845-848.	0.7	0
45	About ErdÃ¶s discrepancy conjecture. Journal of Mathematical Chemistry, 2016, 54, 657-660.	0.7	18
46	A study on the centroid vector of a polyhedron. Journal of Mathematical Chemistry, 2016, 54, 61-71.	0.7	6
47	Quantum polyhedra in LCAO MO theory. Molecular Physics, 2016, 114, 1236-1249.	0.8	12
48	Notes on Quantitative Structure-Properties Relationships (QSPR) Part Four: Quantum Multimolecular Polyhedra, Collective Vectors, Quantum Similarity, and Quantum QSPR Fundamental Equation. Management Studies, 2016, 4, .	0.0	5
49	An isometric representation problem in quantum multimolecular polyhedra and similarity: (2) synisometry. Journal of Mathematical Chemistry, 2015, 53, 1876-1884.	0.7	2
50	Fermi accelerator: A new insight from quantum theory of motion. International Journal of Quantum Chemistry, 2015, 115, 1733-1738.	1.0	4
51	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
52	Quantum polyhedra, definitions, statistics and the construction of a collective quantum similarity index. Journal of Mathematical Chemistry, 2015, 53, 171-182.	0.7	27
53	An isometric representation problem in quantum multimolecular polyhedra and similarity. Journal of Mathematical Chemistry, 2015, 53, 1750-1758.	0.7	17
54	Least squares estimation of unknown molecular properties and quantum QSPR fundamental equation. Journal of Mathematical Chemistry, 2015, 53, 1651-1656.	0.7	12

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55	Coulomb repulsion, point-like nuclear charges, Dirac paradox, soft nuclear charge density and hypermultiplet nuclear repulsion. Journal of Mathematical Chemistry, 2015, 53, 590-603.	0.7	3
56	Six questions on topology in theoretical chemistry. Computational and Theoretical Chemistry, 2015, 1053, 2-16.	1.1	99
57	Multimolecular polyhedra and QSPR. Journal of Mathematical Chemistry, 2014, 52, 1848-1856.	0.7	21
58	A postulate involving quantum mechanical momentum in position space, density function expression of the kinetic energy and Heisenbergâ€™s uncertainty relation. Journal of Mathematical Chemistry, 2014, 52, 1949-1967.	0.7	3
59	A naÃ¯ve geometrical perspective of Fukui functions: definition of Fukui function skew symmetric matrices described on density function sets. Journal of Mathematical Chemistry, 2013, 51, 843-856.	0.7	3
60	Enfolded conformational spaces: definition of the chemical quantum mechanical multiverse under Bornâ€“Oppenheimer approximation. Journal of Mathematical Chemistry, 2013, 51, 1092-1098.	0.7	7
61	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
62	Collective Euclidian distances and quantum similarity. Journal of Mathematical Chemistry, 2013, 51, 338-353.	0.7	20
63	EMP as a similarity measure: a geometric point of view. Journal of Mathematical Chemistry, 2013, 51, 382-389.	0.7	13
64	Position-momentum Heisenberg uncertainty in Gaussian enfoldments of Euclidian space. Journal of Mathematical Chemistry, 2013, 51, 420-426.	0.7	6
65	Function extended spaces. Journal of Mathematical Chemistry, 2013, 51, 660-671.	0.7	3
66	Simple comparison of atomic population and shape atomic populations distributions between two molecular structures with a coherent number of atoms. Journal of Mathematical Chemistry, 2013, 51, 774-784.	0.7	0
67	Variational principle, Hohenbergâ€“Kohn theorem, and density function origin shifts. Journal of Mathematical Chemistry, 2013, 51, 1397-1409.	0.7	8
68	Completely soft molecular electrostatic potentials (CoSMEP) and total density functions. Journal of Mathematical Chemistry, 2013, 51, 1772-1783.	0.7	4
69	On density function coordinate matrix. Journal of Mathematical Chemistry, 2013, 51, 1681-1683.	0.7	4
70	Particle coordinates and discrete molecular description: a geometric point of view on a twofold dimensionality environment. Journal of Mathematical Chemistry, 2013, 51, 1569-1583.	0.7	2
71	Softened electrostatic molecular potentials. Journal of Molecular Graphics and Modelling, 2013, 39, 39-49.	1.3	7
72	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

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73	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
74	Density gradient quantum similarity. , 2012, , .		0
75	Quantum similarity matrices column set as holograms of DF molecular point clouds. Journal of Mathematical Chemistry, 2012, 50, 2339-2341.	0.7	16
76	Stereographic Projection of Density Functions (DF) and the Holographic Electronic Density Theorem (HEDT). Journal of Chemical Theory and Computation, 2012, 8, 854-861.	2.3	7
77	Scaled Euclidian distances: a general dissimilarity index with a suitably defined geometrical foundation. Journal of Mathematical Chemistry, 2012, 50, 734-740.	0.7	17
78	Symmetrical overlap transformations of function basis sets: the LCAO MO and quantum similarity practical cases. Journal of Mathematical Chemistry, 2012, 50, 741-751.	0.7	5
79	On the nature of atomic shell approximation (ASA) electrostatic molecular potentials (EMP). Journal of Mathematical Chemistry, 2012, 50, 981-988.	0.7	10
80	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
81	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
82	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
83	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
84	The relationship between the eigenvalues and eigenvectors of a similarity matrix and its associated CarbÃ³ index matrix. Journal of Mathematical Chemistry, 2011, 49, 6-11.	0.7	2
85	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
86	Logical Kronecker delta deconstruction of the absolute value function and the treatment of absolute deviations. Journal of Mathematical Chemistry, 2011, 49, 619-624.	0.7	4
87	Quantum similarity and discrete representation of molecular sets. Journal of Mathematical Chemistry, 2011, 49, 1558-1572.	0.7	25
88	The general Gaussian product theorem. Journal of Mathematical Chemistry, 2011, 49, 1769-1784.	0.7	15
89	Quantum similarity, volume functions and generalized CarbÃ³ indices. Journal of Mathematical Chemistry, 2011, 49, 2109-2115.	0.7	14
90	n-Dimensional Euclidean space Gaussian enfoldment. Journal of Mathematical Chemistry, 2011, 49, 2231-2243.	0.7	7

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91	Geometry of n-dimensional Euclidean space Gaussian enfoldments. Journal of Mathematical Chemistry, 2011, 49, 2244-2249.	0.7	10
92	Communications on quantum similarity, part 3: A geometricâ€quantum similarity molecular superposition algorithm. Journal of Computational Chemistry, 2011, 32, 582-599.	1.5	48
93	Definition of norm coherent generalized scalar products and quantum similarity. Journal of Mathematical Chemistry, 2010, 47, 331-344.	0.7	19
94	A monodimensional scientific performance measure: the h index, can be substituted by simple multidimensional descriptors?. Journal of Mathematical Chemistry, 2010, 47, 548-550.	0.7	4
95	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
96	Commentaries on quantum similarity (1): Density gradient quantum similarity. Journal of Computational Chemistry, 2010, 31, 2195-2212.	1.5	42
97	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
98	LCAO MO first order density functions: Partition in monocentric and bicentric terms, reciprocal MO spaces, invariant transformations and Euclidian atomic populations. Computational and Theoretical Chemistry, 2010, 943, 32-41.	1.5	4
99	Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284.	1.5	76
100	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
101	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
102	Expectation value averages of size consistent hermitian operators and the definition of Fukui functions. International Journal of Quantum Chemistry, 2009, 109, 2356-2364.	1.0	2
103	Quantum Similarity and Quantum Quantitative Structure-Properties Relationships (QQSPR). , 2009, , 7422-7480.		24
104	Molecular Quantum Similarity. , 2009, , .		3
105	Mathematical aspects of the LCAO MO first order density function (3): A general localization procedure. Journal of Mathematical Chemistry, 2008, 43, 1069-1075.	0.7	7
106	Mathematical aspects of the LCAO MO first order density function (1): atomic partition, metric structure and practical applications. Journal of Mathematical Chemistry, 2008, 43, 1076-1101.	0.7	8
107	Mathematical aspects of the LCAO MO first order density function (2): Relationships between density functions. Journal of Mathematical Chemistry, 2008, 43, 1102-1118.	0.7	7
108	A quantum similarity matrix (QSM) Aufbau procedure. Journal of Mathematical Chemistry, 2008, 44, 228-234.	0.7	16

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109	Smooth function topological structure descriptors based on graph-spectra. Journal of Mathematical Chemistry, 2008, 44, 373-378.	0.7	13
110	Riemannian three dimensional molecular spaces. Journal of Mathematical Chemistry, 2008, 44, 286-300.	0.7	7
111	Diagonal coefficient representation of density functions and quantum similarity measures. Journal of Mathematical Chemistry, 2008, 44, 621-627.	0.7	11
112	Molecular quantum similarity measures in Minkowski metric vector semispaces. Journal of Mathematical Chemistry, 2008, 44, 628-636.	0.7	27
113	A new insight on the quantum quantitative structureâ€properties relationships. International Journal of Quantum Chemistry, 2008, 108, 1721-1734.	1.0	21
114	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
115	Critical analysis and extension of the Hirshfeld atoms in molecules. Journal of Chemical Physics, 2007, 126, 144111.	1.2	577
116	Critical thoughts on computing atom condensed Fukui functions. Journal of Chemical Physics, 2007, 127, 034102.	1.2	162
117	Comment on â€œChemoselectives in Acetalization, Thioacetalization, Oxathioacetalization and Azathioacetalizationâ€• Journal of Physical Chemistry A, 2007, 111, 2640-2640.	1.1	3
118	Aromaticity in linear polyacenes: Generalized population analysis and molecular quantum similarity approach. Journal of Computational Chemistry, 2007, 28, 152-160.	1.5	51
119	Unrevealed structural requirements for auxin-like molecules by theoretical and experimental evidences. Phytochemistry, 2007, 68, 237-250.	1.4	20
120	Solutions to the Quantum QSPR problem in molecular spaces. Theoretical Chemistry Accounts, 2007, 118, 673-679.	0.5	24
121	On Einsteinâ€“Podolskyâ€“Rosen Paradox. Journal of Mathematical Chemistry, 2007, 41, 209-215.	0.7	5
122	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
123	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
124	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
125	Modelling Toxicity using Molecular Quantum Similarity Measures. QSAR and Combinatorial Science, 2006, 25, 579-589.	1.5	38
126	A Discussion on the Einsteinâ€“Podolskiâ€“Rosen (EPR) Effect* in a Unique Wavefunction Quantum Mechanical Framework. Journal of Mathematical Chemistry, 2006, 39, 267-279.	0.7	2

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127	Generation of Molecular Fields, Quantum Similarity Measures and Related Questions. Journal of Mathematical Chemistry, 2006, 39, 495-510.	0.7	9
128	Descriptors and Probability Distributions in MO Theory: Weighted Mulliken Matrices and Molecular Quantum Similarity Measures. Journal of Mathematical Chemistry, 2006, 39, 551-591.	0.7	7
129	Select-divide-and-conquer method for large-scale configuration interaction. Journal of Chemical Physics, 2006, 125, 014108.	1.2	23
130	Maximal probability domains in linear molecules. Journal of Computational Chemistry, 2005, 26, 455-460.	1.5	36
131	Geometric and electronic similarities between transition structures for electrocyclizations and sigmatropic hydrogen shifts. Theoretical Chemistry Accounts, 2005, 113, 205-211.	0.5	6
132	Molecular quantum similarity using conceptual DFT descriptors. Journal of Chemical Sciences, 2005, 117, 425-435.	0.7	29
133	Deduction of Heisenberg relations and SchrÃ¶dinger equation through the structure of NÂ-dimensional parameterized metric vector spaces. Journal of Mathematical Chemistry, 2005, 38, 89-101.	0.7	4
134	Molecular Nuclear Fields: A NaÃ¯ve Perspective. Journal of Mathematical Chemistry, 2005, 38, 671-676.	0.7	7
135	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
136	Mathematical Elements of Quantum Electronic Density Functions. Advances in Quantum Chemistry, 2005, , 121-207.	0.4	15
137	Heisenbergâ€™s Relations in Discrete N-Dimensional Parameterized Metric Vector Spaces. Journal of Mathematical Chemistry, 2004, 36, 41-54.	0.7	7
138	Infinite-Dimensional Time Vectors as Background Building Blocks of a Spaceâ€“Time Frame Structure. Journal of Mathematical Chemistry, 2004, 36, 75-81.	0.7	8
139	A Mathematical Discussion on Density and Shape Functions, Vector Semispaces and Related Questions. Journal of Mathematical Chemistry, 2004, 36, 191-200.	0.7	61
140	A General Procedure to Obtain Quantum Mechanical Charge and Bond Order Molecular Parameters. Journal of Mathematical Chemistry, 2004, 36, 201-210.	0.7	30
141	Quantum Mechanical Basis for Mulliken Population Analysis. Journal of Mathematical Chemistry, 2004, 36, 231-239.	0.7	74
142	Non-linear Terms & Variational Approach in Quantum QSPR. Journal of Mathematical Chemistry, 2004, 36, 241-260.	0.7	18
143	Discussion on the variable Wolfsberg-Helmholtz parameter, a new simplified LÃ¶wdin transformation and the characteristic structure of the transformed EHT Hamiltonian matrices. International Journal of Quantum Chemistry, 2004, 98, 26-32.	1.0	0
144	Estimation of infinite dilution activity coefficients of organic compounds in water with neural classifiers. AICHE Journal, 2004, 50, 1315-1343.	1.8	26

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145	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
146	Similarity approach to QSAR. International Journal of Pharmaceutics, 2004, 269, 51-60.	2.6	19
147	Title is missing!. Journal of Mathematical Chemistry, 2003, 33, 227-244.	0.7	12
148	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
149	Title is missing!. Journal of Mathematical Chemistry, 2003, 34, 75-82.	0.7	4
150	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
151	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
152	Molecular Quantum Similarity Analysis of Estrogenic Activity.. ChemInform, 2003, 34, no.	0.1	0
153	Quality of Approximate Electron Densities and Internal Consistency of Molecular Alignment Algorithms in Molecular Quantum Similarity.. ChemInform, 2003, 34, no.	0.1	0
154	Classification of reaction pathways via momentumâ€“space and quantum molecular similarity measures. Chemical Physics Letters, 2003, 367, 207-213.	1.2	12
155	Rational modelling of the voltage-dependent K+ channel inactivation by aminopyridines. Biophysical Chemistry, 2003, 104, 417-427.	1.5	20
156	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
157	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
158	Molecular Quantum Similarity-Based QSARs for Binding Affinities of Several Steroid SetsJ. Chem. Inf. Comput. Sci.42, 1185â˜'1193 (2002). Journal of Chemical Information and Computer Sciences, 2003, 43, 1335-1336.	2.8	2
159	Molecular Quantum Similarity Analysis of Estrogenic Activity. Journal of Chemical Information and Computer Sciences, 2003, 43, 1166-1176.	2.8	45
160	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
161	Molecular Quantum Similarity Matrix Based Clustering of Molecules Using Dendrograms. Journal of Chemical Information and Computer Sciences, 2003, 43, 170-177.	2.8	30
162	Negative Fukui functions: New insights based on electronegativity equalization. Journal of Chemical Physics, 2003, 118, 4349-4356.	1.2	114

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163	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
164	Structureâ€”property relationships and momentum space quantities: Hammett Ïƒâ€”constants. Molecular Physics, 2003, 101, 3159-3162.	0.8	20
165	DENSITY FUNCTIONS AND GENERATING WAVE FUNCTIONS. , 2002, , 401-412.		9
166	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
167	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
168	Modeling Large Macromolecular Structures Using Promolecular Densities. Journal of Chemical Information and Computer Sciences, 2002, 42, 847-852.	2.8	26
169	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
170	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
171	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
172	Algebraic relationships between conceptual DFT quantities and the electronegativity equalization hardness matrix. Chemical Physics Letters, 2002, 364, 357-362.	1.2	19
173	Molecular Quantum Similarity and the Fundamentals of QSAR. Accounts of Chemical Research, 2002, 35, 289-295.	7.6	99
174	Title is missing!. Journal of Mathematical Chemistry, 2002, 32, 201-223.	0.7	45
175	Modeling Large Macromolecular Structures Using Promolecular Densities.. ChemInform, 2002, 33, 234-234.	0.1	0
176	Molecular Quantum Similarityâ€Based QSARs for Binding Affinities of Several Steroid Sets.. ChemInform, 2002, 33, 214-214.	0.1	0
177	Identification of Active Molecular Sites Using Quantum-Self-Similarity Measures. Journal of Chemical Information and Computer Sciences, 2001, 41, 978-991.	2.8	39
178	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
179	Theoretical and computational aspects of extended wave functions. International Journal of Quantum Chemistry, 2001, 84, 331-337.	1.0	2
180	TGSA: A molecular superposition program based on topo-geometrical considerations. Journal of Computational Chemistry, 2001, 22, 255-263.	1.5	70

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181	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
182	Title is missing!. Journal of Mathematical Chemistry, 2001, 30, 227-245.	0.7	31
183	Generalized one-electron spin functions and self-similarity measures. Journal of Mathematical Chemistry, 2001, 29, 41-45.	0.7	5
184	Title is missing!. , 2001, 29, 3-20.		5
185	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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