Ramon Carb-Dorca i Carr

List of Publications by Year in Descending Order

282 papers	6,808 citations	42 h-index	67 g-index
300 ext. papers	7,375 ext. citations	2.7 avg, IF	6.28 L-index

#	Paper	IF	Citations
282	Average energy and quantum similarity of a time dependent quantum system subject to Pöschl-Teller potential. *Journal of Mathematical Chemistry*, **2022**, 60, 1-21	2.1	1
281	A naïve HMO study of the casimir effect. *Journal of Mathematical Chemistry*, **2022**, 60, 581	2.1	0
280	Determination of unknown molecular properties in molecular spaces. *Journal of Mathematical Chemistry*, **2022**, 60, 353	2.1	0
279	Generalized scalar products in Minkowski metric spaces. *Journal of Mathematical Chemistry*, **2021**, 59, 1029-1045	2.1	4
278	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	2.1	0
277	Extended Minkowski spaces, zero norms, and Minkowski hypersurfaces. *Journal of Mathematical Chemistry*, **2021**, 59, 1875-1879	2.1	2
276	Extension of Fermat's last theorem in Minkowski natural spaces. *Journal of Mathematical Chemistry*, **2021**, 59, 1851-1863	2.1	
275	About the construction of probability hypercubes. *Journal of Mathematical Chemistry*, **2021**, 59, 1151-1154	2.1	
274	An HPC hybrid parallel approach to the experimental analysis of Fermat's theorem extension to arbitrary dimensions on heterogeneous computer systems. *Journal of Supercomputing*, **2021**, 77, 11328-11352	2.5	2
273	Fuzzy Hypercubes and their time-like evolution. *Journal of Mathematical Chemistry*, **2020**, 58, 1337-1344	2.1	4
272	Cantor-like transfinite sequences and Gödel-like incompleteness revealed by means of Mersenne transfinite dimensional boolean hypercube concatenation. *Journal of Mathematical Chemistry*, **2020**, 58, 1-5	2.1	7
271	A quantum similarity discussion about Einstein-Podolsky-Rosen (EPR) paradox in Gaussian enfolded spaces. *Journal of Mathematical Chemistry*, **2020**, 58, 1815-1827	2.1	4
270	Hypercubes defined on n-ary sets, the Erdős-Faber-Lovász conjecture on graph coloring, and the description spaces of polypeptides and RNA. *Journal of Mathematical Chemistry*, **2019**, 57, 2182-2194	2.1	8
269	Vector spaces defined over the unit interval. *Journal of Mathematical Chemistry*, **2019**, 57, 691-693	2.1	
268	Universal transformation and non-linear connection between experimental and calculated property vectors in QSPR. *Journal of Mathematical Chemistry*, **2019**, 57, 1075-1087	2.1	2
267	Divagations about the periodic table: Boolean hypercube and quantum similarity connections. *Journal of Computational Chemistry*, **2019**, 40, 2653-2663	3.5	15
266	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70

265	Transformation of boolean hypercube vertices into unit interval elements: QSPR workout consequences. *Journal of Mathematical Chemistry*, **2019**, 57, 694-696	2.1	5
264	Role of the structure of Boolean hypercubes when used as vectors in natural (Boolean) vector semispaces. *Journal of Mathematical Chemistry*, **2019**, 57, 697-700	2.1	7
263	Toward a universal quantum QSPR operator. *International Journal of Quantum Chemistry*, **2018**, 118, e25602	2.1	11
262	Boolean Hypercubes as time representation holders. *Journal of Mathematical Chemistry*, **2018**, 56, 1349-1352	2.1	10
261	DNA, unnatural base pairs and hypercubes. *Journal of Mathematical Chemistry*, **2018**, 56, 1353-1356	2.1	17
260	Thermal scaling of electronic energy expressions. *Journal of Mathematical Chemistry*, **2018**, 56, 979-981	2.1	
259	Atomic thermal voltage population distributions. *Journal of Mathematical Chemistry*, **2018**, 56, 1357-1359	2.1	
258	Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. *Structural Chemistry*, **2018**, 29, 33-38	1.8	47
257	Boolean hypercubes and the structure of vector spaces. *Journal of Mathematical Sciences and Modelling*, **2018**, 1, 1-14	3	6
256	Statistical-like signature of molecular basis sets. *Journal of Molecular Modeling*, **2018**, 24, 256	2	1
255	A theorem on the Gram matrix of a polyhedron. *Journal of Mathematical Chemistry*, **2017**, 55, 79-97	2.1	5
254	Refinement of a generalized Fermat last theorem conjecture in natural vector spaces. *Journal of Mathematical Chemistry*, **2017**, 55, 1869-1877	2.1	9
253	Natural Vector Spaces (inward power and Minkowski norm of a Natural Vector, Natural Boolean Hypercubes) and a Fermat Last Theorem conjecture. *Journal of Mathematical Chemistry*, **2017**, 55, 914-940	2.1	22
252	A study on the centroid vector of a polyhedron. *Journal of Mathematical Chemistry*, **2016**, 54, 61-71	2.1	2
251	Quantum polyhedra in LCAO MO theory. *Molecular Physics*, **2016**, 114, 1236-1249	1.7	8
250	Time vectors and particle swarms defined as polyhedra in spherically enfolded spaces. *Journal of Mathematical Chemistry*, **2016**, 54, 1751-1757	2.1	7
249	A study on Goldbach conjecture. *Journal of Mathematical Chemistry*, **2016**, 54, 1798-1809	2.1	12
248	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	2.1	

247	About Erdős discrepancy conjecture. *Journal of Mathematical Chemistry*, **2016**, 54, 657-660	2.1	16
246	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,	1.3	3
245	Aromaticity, quantum multimolecular polyhedra, and quantum QSPR fundamental equation. *Journal of Computational Chemistry*, **2016**, 37, 78-82	3.5	10
244	On the nature of the collective quantum mechanical description of molecular atoms and bonds. *Journal of Mathematical Chemistry*, **2016**, 54, 1440-1446	2.1	4
243	N-dimensional Boolean hypercubes and the goldbach conjecture. *Journal of Mathematical Chemistry*, **2016**, 54, 1213-1220	2.1	21
242	Quantum polyhedra, definitions, statistics and the construction of a collective quantum similarity index. *Journal of Mathematical Chemistry*, **2015**, 53, 171-182	2.1	22
241	An isometric representation problem in quantum multimolecular polyhedra and similarity. *Journal of Mathematical Chemistry*, **2015**, 53, 1750-1758	2.1	13
240	Least squares estimation of unknown molecular properties and quantum QSPR fundamental equation. *Journal of Mathematical Chemistry*, **2015**, 53, 1651-1656	2.1	8
239	Coulomb repulsion, point-like nuclear charges, Dirac paradox, soft nuclear charge density and hypermultiplet nuclear repulsion. *Journal of Mathematical Chemistry*, **2015**, 53, 590-603	2.1	1
238	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
237	An isometric representation problem in quantum multimolecular polyhedra and similarity: (2) synisometry. *Journal of Mathematical Chemistry*, **2015**, 53, 1876-1884	2.1	1
236	Fermi accelerator: A new insight from quantum theory of motion. *International Journal of Quantum Chemistry*, **2015**, 115, 1733-1738	2.1	3
235	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	7.9	22
234	Multimolecular polyhedra and QSPR. *Journal of Mathematical Chemistry*, **2014**, 52, 1848-1856	2.1	19
233	A postulate involving quantum mechanical momentum in position space, density function expression of the kinetic energy and Heisenberg uncertainty relation. *Journal of Mathematical Chemistry*, **2014**, 52, 1949-1967	2.1	3
232	A naïve 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	2.1	3
231	Enfolded conformational spaces: definition of the chemical quantum mechanical multiverse under Born–Oppenheimer approximation. *Journal of Mathematical Chemistry*, **2013**, 51, 1092-1098	2.1	5
230	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	2.1	17

229	Collective Euclidian distances and quantum similarity. *Journal of Mathematical Chemistry*, **2013**, 51, 338-353	2.1	16
228	EMP as a similarity measure: a geometric point of view. *Journal of Mathematical Chemistry*, **2013**, 51, 382-389	2.1	10
227	Position-momentum Heisenberg uncertainty in Gaussian enfoldments of Euclidian space. *Journal of Mathematical Chemistry*, **2013**, 51, 420-426	2.1	5
226	Function extended spaces. *Journal of Mathematical Chemistry*, **2013**, 51, 660-671	2.1	2
225	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	2.1	
224	Variational principle, Hohenberg-Kohn theorem, and density function origin shifts. *Journal of Mathematical Chemistry*, **2013**, 51, 1397-1409	2.1	8
223	Completely soft molecular electrostatic potentials (CoSMEP) and total density functions. *Journal of Mathematical Chemistry*, **2013**, 51, 1772-1783	2.1	3
222	On density function coordinate matrix. *Journal of Mathematical Chemistry*, **2013**, 51, 1681-1683	2.1	4
221	Particle coordinates and discrete molecular description: a geometric point of view on a twofold dimensionality environment. *Journal of Mathematical Chemistry*, **2013**, 51, 1569-1583	2.1	2
220	Softened electrostatic molecular potentials. *Journal of Molecular Graphics and Modelling*, **2013**, 39, 39-49	2.8	6
219	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	2.1	7
218	Notes on quantitative structure-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, 766-79	3.5	21
217	Shells, point cloud huts, generalized scalar products, cosines and similarity tensor representations in vector semispaces. *Journal of Mathematical Chemistry*, **2012**, 50, 210-219	2.1	36
216	Quantum similarity matrices column set as holograms of DF molecular point clouds. *Journal of Mathematical Chemistry*, **2012**, 50, 2339-2341	2.1	14
215	Stereographic Projection of Density Functions (DF) and the Holographic Electronic Density Theorem (HEDT). *Journal of Chemical Theory and Computation*, **2012**, 8, 854-61	6.4	7
214	Scaled Euclidian distances: a general dissimilarity index with a suitably defined geometrical foundation. *Journal of Mathematical Chemistry*, **2012**, 50, 734-740	2.1	16
213	Symmetrical overlap transformations of function basis sets: the LCAO MO and quantum similarity practical cases. *Journal of Mathematical Chemistry*, **2012**, 50, 741-751	2.1	2
212	On the nature of atomic shell approximation (ASA) electrostatic molecular potentials (EMP). *Journal of Mathematical Chemistry*, **2012**, 50, 981-988	2.1	7

211	Centroid origin shift of quantum object sets and molecular point clouds description and element comparisons. *Journal of Mathematical Chemistry*, **2012**, 50, 1161-1178	2.1	23
210	The Fukui matrix: a simple approach to the analysis of the Fukui function and its positive character. *Physical Chemistry Chemical Physics*, **2011**, 13, 6110-5	3.6	44
209	Construction of coherent nano quantitative structure-properties relationships (nano-QSPR) models and catastrophe theory. *SAR and QSAR in Environmental Research*, **2011**, 22, 661-5	3.5	21
208	The relationship between the eigenvalues and eigenvectors of a similarity matrix and its associated Carbó index matrix. *Journal of Mathematical Chemistry*, **2011**, 49, 6-11	2.1	2
207	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	2.1	13
206	Logical Kronecker delta deconstruction of the absolute value function and the treatment of absolute deviations. *Journal of Mathematical Chemistry*, **2011**, 49, 619-624	2.1	3
205	Quantum similarity and discrete representation of molecular sets. *Journal of Mathematical Chemistry*, **2011**, 49, 1558-1572	2.1	23
204	The general Gaussian product theorem. *Journal of Mathematical Chemistry*, **2011**, 49, 1769-1784	2.1	11
203	Quantum similarity, volume functions and generalized Carbó indices. *Journal of Mathematical Chemistry*, **2011**, 49, 2109-2115	2.1	13
202	n-Dimensional Euclidean space Gaussian enfoldment. *Journal of Mathematical Chemistry*, **2011**, 49, 2231-2243	2.1	7
201	Geometry of n-dimensional Euclidean space Gaussian enfoldments. *Journal of Mathematical Chemistry*, **2011**, 49, 2244-2249	2.1	9
200	Communications on quantum similarity, part 3: a geometric-quantum similarity molecular superposition algorithm. *Journal of Computational Chemistry*, **2011**, 32, 582-99	3.5	41
199	Definition of norm coherent generalized scalar products and quantum similarity. *Journal of Mathematical Chemistry*, **2010**, 47, 331-344	2.1	15
198	A monodimensional scientific performance measure: the h index, can be substituted by simple multidimensional descriptors?. *Journal of Mathematical Chemistry*, **2010**, 47, 548-550	2.1	3
197	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	2.1	14
196	Commentaries on quantum similarity (1): Density gradient quantum similarity. *Journal of Computational Chemistry*, **2010**, 31, 2195-212	3.5	39
195	Communications on quantum similarity (2): A geometric discussion on holographic electron density theorem and confined quantum similarity measures. *Journal of Computational Chemistry*, **2010**, 31, 2452-62	3.5	9
194	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		4

193	Modeling the structure-property relationships of nanoneedles: A journey toward nanomedicine. *Journal of Computational Chemistry*, **2009**, 30, 275-84	3.5	71
192	Notes on quantitative structure-properties relationships (QSPR) (1): A discussion on a QSPR dimensionality paradox (QSPR DP) and its quantum resolution. *Journal of Computational Chemistry*, **2009**, 30, 1146-59	3.5	26
191	Notes on quantitative structure-properties relationships (QSPR) part 2: the role of the number of atoms as a molecular descriptor. *Journal of Computational Chemistry*, **2009**, 30, 2099-104	3.5	10
190	Expectation value averages of size consistent hermitian operators and the definition of Fukui functions. *International Journal of Quantum Chemistry*, **2009**, 109, 2356-2364	2.1	2
189	Molecular Quantum Similarity **2009**,		3
188	Mathematical aspects of the LCAO MO first order density function (3): A general localization procedure. *Journal of Mathematical Chemistry*, **2008**, 43, 1069-1075	2.1	6
187	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	2.1	7
186	Mathematical aspects of the LCAO MO first order density function (2): Relationships between density functions. *Journal of Mathematical Chemistry*, **2008**, 43, 1102-1118	2.1	6
185	A quantum similarity matrix (QSM) Aufbau procedure. *Journal of Mathematical Chemistry*, **2008**, 44, 228-234	2.1	13
184	Smooth function topological structure descriptors based on graph-spectra. *Journal of Mathematical Chemistry*, **2008**, 44, 373-378	2.1	10
183	Riemannian three dimensional molecular spaces. *Journal of Mathematical Chemistry*, **2008**, 44, 286-300	2.1	6
182	Diagonal coefficient representation of density functions and quantum similarity measures. *Journal of Mathematical Chemistry*, **2008**, 44, 621-627	2.1	8
181	Molecular quantum similarity measures in Minkowski metric vector semispaces. *Journal of Mathematical Chemistry*, **2008**, 44, 628-636	2.1	19
180	A new insight on the quantum quantitative structure-properties relationships. *International Journal of Quantum Chemistry*, **2008**, 108, 1721-1734	2.1	17
179	Comment on "Chemoselectives in acetalization, thioacetalization, oxathioacetalization and azathioacetalization". *Journal of Physical Chemistry A*, **2007**, 111, 2640	2.8	3
178	Aromaticity in linear polyacenes: generalized population analysis and molecular quantum similarity approach. *Journal of Computational Chemistry*, **2007**, 28, 152-60	3.5	46
177	Unrevealed structural requirements for auxin-like molecules by theoretical and experimental evidences. *Phytochemistry*, **2007**, 68, 237-50	4	15
176	Solutions to the Quantum QSPR problem in molecular spaces. *Theoretical Chemistry Accounts*, **2007**, 118, 673-679	1.9	18

175	On Einstein-Podolsky-Rosen Paradox. *Journal of Mathematical Chemistry*, **2007**, 41, 209-215	2.1	3
174	About the prediction of molecular properties using the fundamental Quantum QSPR (QQSPR) equation. *SAR and QSAR in Environmental Research*, **2007**, 18, 265-84	3.5	21
173	Critical analysis and extension of the Hirshfeld atoms in molecules. *Journal of Chemical Physics*, **2007**, 126, 144111	3.9	484
172	Critical thoughts on computing atom condensed Fukui functions. *Journal of Chemical Physics*, **2007**, 127, 034102	3.9	128
171	Select-divide-and-conquer method for large-scale configuration interaction. *Journal of Chemical Physics*, **2006**, 125, 014108	3.9	20
170	Electron delocalization and aromaticity in linear polyacenes: atoms in molecules multicenter delocalization index. *Journal of Physical Chemistry A*, **2006**, 110, 7642-8	2.8	159
169	Coulomb and overlap self-similarities: a comparative selectivity analysis of structure-function relationships for auxin-like molecules. *Journal of Chemical Information and Modeling*, **2006**, 46, 1751-62	6.1	25
168	Toward an alternative hardness kernel matrix structure in the Electronegativity Equalization Method (EEM). *Journal of Chemical Information and Modeling*, **2006**, 46, 1657-65	6.1	13
167	Modelling Toxicity using Molecular Quantum Similarity Measures. *QSAR and Combinatorial Science*, **2006**, 25, 579-589		30
166	A Discussion on the Einstein-Podolski-Rosen (EPR) Effect* in a Unique Wavefunction Quantum Mechanical Framework. *Journal of Mathematical Chemistry*, **2006**, 39, 267-279	2.1	2
165	Generation of Molecular Fields, Quantum Similarity Measures and Related Questions. *Journal of Mathematical Chemistry*, **2006**, 39, 495-510	2.1	7
164	Descriptors and Probability Distributions in MO Theory: Weighted Mulliken Matrices and Molecular Quantum Similarity Measures. *Journal of Mathematical Chemistry*, **2006**, 39, 551-591	2.1	6
163	Mathematical Elements of Quantum Electronic Density Functions. *Advances in Quantum Chemistry*, **2005**, 121-207	1.4	11
162	Maximal probability domains in linear molecules. *Journal of Computational Chemistry*, **2005**, 26, 455-60	3.5	33
161	Geometric and electronic similarities between transition structures for electrocyclizations and sigmatropic hydrogen shifts. *Theoretical Chemistry Accounts*, **2005**, 113, 205-211	1.9	5
160	Molecular quantum similarity using conceptual DFT descriptors. *Journal of Chemical Sciences*, **2005**, 117, 425-435	1.8	25
159	Deduction of Heisenberg relations and Schrödinger equation through the structure of N -dimensional parameterized metric vector spaces. *Journal of Mathematical Chemistry*, **2005**, 38, 89-101	2.1	4
158	Molecular Nuclear Fields: A Naïve Perspective. *Journal of Mathematical Chemistry*, **2005**, 38, 671-676	2.1	6

157	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	2.1	38
156	Heisenberg Relations in Discrete N-Dimensional Parameterized Metric Vector Spaces. *Journal of Mathematical Chemistry*, **2004**, 36, 41-54	2.1	5
155	Infinite-Dimensional Time Vectors as Background Building Blocks of a Space Time Frame Structure. *Journal of Mathematical Chemistry*, **2004**, 36, 75-81	2.1	6
154	A Mathematical Discussion on Density and Shape Functions, Vector Semispaces and Related Questions. *Journal of Mathematical Chemistry*, **2004**, 36, 191-200	2.1	54
153	A General Procedure to Obtain Quantum Mechanical Charge and Bond Order Molecular Parameters. *Journal of Mathematical Chemistry*, **2004**, 36, 201-210	2.1	29
152	Quantum Mechanical Basis for Mulliken Population Analysis. *Journal of Mathematical Chemistry*, **2004**, 36, 231-239	2.1	55
151	Non-linear Terms & Variational Approach in Quantum QSPR. *Journal of Mathematical Chemistry*, **2004**, 36, 241-260	2.1	13
150	Discussion on the variable Wolfsberg Helmholtz parameter, a new simplified Lwdin transformation and the characteristic structure of the transformed EHT Hamiltonian matrices. *International Journal of Quantum Chemistry*, **2004**, 98, 26-32	2.1	
149	Estimation of infinite dilution activity coefficients of organic compounds in water with neural classifiers. *AICHE Journal*, **2004**, 50, 1315-1343	3.6	20
148	TGSA-Flex: Extending the capabilities of the Topo-Geometrical Superposition Algorithm to handle flexible molecules. *Journal of Computational Chemistry*, **2004**, 25, 153-9	3.5	19
147	Similarity approach to QSAR. Application to antimycobacterial benzoxazines. *International Journal of Pharmaceutics*, **2004**, 269, 51-60	6.5	17
146	About Some Questions Relative to the Arbitrariness of Signs: Their Possible Consequences in Matrix Signatures Definition and Quantum Chemical Applications. *Journal of Mathematical Chemistry*, **2003**, 33, 227-244	2.1	8
145	Negative and Infinite Fukui Functions: The Role of Diagonal Dominance in the Hardness Matrix. *Journal of Mathematical Chemistry*, **2003**, 34, 67-74	2.1	52
144	Analysis of a General Theorem Concerning Two Non-Commuting Hermitian Matrices: Quantum Mechanical Implications for Ground and Excited States. *Journal of Mathematical Chemistry*, **2003**, 34, 75-82	2.1	2
143	Fast calculation of quantum chemical molecular descriptors from the electronegativity equalization method. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 422-8		27
142	Chemical structures from the analysis of domain-averaged Fermi holes: multiple metal-metal bonding in transition metal compounds. *Journal of Computational Chemistry*, **2003**, 24, 1829-38	3.5	37
141	Classification of reaction pathways via momentum space and quantum molecular similarity measures. *Chemical Physics Letters*, **2003**, 367, 207-213	2.5	9
140	Rational modelling of the voltage-dependent K+ channel inactivation by aminopyridines. *Biophysical Chemistry*, **2003**, 104, 417-27	3.5	18

139	Applications of inward matrix products and matrix wave functions to Hückel MO theory, Slater extended wave functions, spin extended functions, and Hartree method. *International Journal of Quantum Chemistry*, **2003**, 91, 607-617	2.1	15
138	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, 2033-8		23
137	Molecular Quantum Similarity-Based QSARs for Binding Affinities of Several Steroid Sets J. Chem. Inf. Comput. Sci.42, 1185-1193 (2002). *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1335-1336		1
136	Molecular quantum similarity analysis of estrogenic activity. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1166-76		36
135	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, 1208-17		30
134	Molecular quantum similarity matrix based clustering of molecules using dendrograms. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 170-7		26
133	Negative Fukui functions: New insights based on electronegativity equalization. *Journal of Chemical Physics*, **2003**, 118, 4349-4356	3.9	99
132	Quantum similarity superposition algorithm (QSSA): a consistent scheme for molecular alignment and molecular similarity based on quantum chemistry. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1143-50		38
131	Structure-property relationships and momentum space quantities: Hammett constants. *Molecular Physics*, **2003**, 101, 3159-3162	1.7	16
130	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	2.1	39
129	Fundamental quantum QSAR (Q2SAR) equation: extensions, nonlinear terms, and generalizations within extended Hilbert-Sobolev spaces. *International Journal of Quantum Chemistry*, **2002**, 88, 167-182	2.1	16
128	Algebraic relationships between conceptual DFT quantities and the electronegativity equalization hardness matrix. *Chemical Physics Letters*, **2002**, 364, 357-362	2.5	18
127	Molecular quantum similarity and the fundamentals of QSAR. *Accounts of Chemical Research*, **2002**, 35, 289-95	24.3	78
126	Shell Partition and Metric Semispaces: Minkowski Norms, Root Scalar Products, Distances and Cosines of Arbitrary Order. *Journal of Mathematical Chemistry*, **2002**, 32, 201-223	2.1	38
125	DENSITY FUNCTIONS AND GENERATING WAVE FUNCTIONS **2002**, 401-412		6
124	Using molecular quantum similarity measures under stochastic transformation to describe physical properties of molecular systems. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 317-25		9
123	Molecular basis of linear free energy relationships. The nature of inductive effect in aliphatic series. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 564-70		18
122	Modeling large macromolecular structures using promolecular densities. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 847-52		20

121	Molecular quantum similarity-based QSARs for binding affinities of several steroid sets. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 1185-93		13
120	Application of promolecular ASA densities to graphical representation of density functions of macromolecular systems. *Journal of Molecular Graphics and Modelling*, **2001**, 19, 343-8	2.8	21
119	Theoretical and computational aspects of extended wave functions. *International Journal of Quantum Chemistry*, **2001**, 84, 331-337	2.1	1
118	TGSA: A molecular superposition program based on topo-geometrical considerations. *Journal of Computational Chemistry*, **2001**, 22, 255-263	3.5	58
117	Antimalarial activity of synthetic 1,2,4-trioxanes and cyclic peroxy ketals, a quantum similarity study. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 1053-63	4.2	12
116	Inward Matrix Product Algebra and Calculus as Tools to Construct Space□Time Frames of Arbitrary Dimensions. *Journal of Mathematical Chemistry*, **2001**, 30, 227-245	2.1	23
115	Generalized one-electron spin functions and self-similarity measures. *Journal of Mathematical Chemistry*, **2001**, 29, 41-45	2.1	4
114	Extended Sobolev and Hilbert spaces and approximate stationary solutions for electronic systems within the non-linear Schr□inger equation **2001**, 29, 3-20		3
113	Structure-toxicity relationships of polycyclic aromatic hydrocarbons using molecular quantum similarity. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 67-80	4.2	26
112	Inward matrix products: extensions and applications to quantum mechanical foundations of QSAR. *Computational and Theoretical Chemistry*, **2001**, 537, 41-54		46
111	Molecular Quantum Similarity Measures as Descriptors for Quantum QSAR. *Polycyclic Aromatic Compounds*, **2001**, 19, 51-71	1.3	5
110	Identification of active molecular sites using quantum-self-similarity measures. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 978-91		35
109	Quantum Molecular Similarity: Theory and Applications to the Evaluation of Molecular Properties, Biological Activities and Toxicity. *Mathematical and Computational Chemistry*, **2001**, 187-320		20
108	Extended density functions. *Advances in Quantum Chemistry*, **2000**, 38, 1-63	1.4	12
107	General trends in atomic and nuclear quantum similarity measures. *International Journal of Quantum Chemistry*, **2000**, 77, 685-692	2.1	27
106	Stochastic transformation of quantum similarity matrices and their use in quantum QSAR (QQSAR) models. *International Journal of Quantum Chemistry*, **2000**, 79, 163-177	2.1	28
105	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	2.1	15
104	Icosahedral symmetry structures with open-shell electronic configuration hN (N=1□).. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2000**, 267, 370-378	2.3	12

103	Quantum mechanical origin of QSAR: theory and applications. *Computational and Theoretical Chemistry*, **2000**, 504, 181-228		52
102	Inward matrix products, generalised density functions and Rayleigh-Schrödinger perturbation theory. *Computational and Theoretical Chemistry*, **2000**, 501-502, 173-176		17
101	Quantum QSAR and the eigensystems of stochastic quantum similarity matrices. *Journal of Mathematical Chemistry*, **2000**, 27, 357-376	2.1	12
100	Use of electron-electron repulsion energy as a molecular descriptor in QSAR and QSPR studies. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 477-85	4.2	28
99	Quantum chemistry, Sobolev spaces and SCF. *Journal of Mathematical Chemistry*, **2000**, 28, 59-70	2.1	2
98	A discussion on an apparent MO theory paradox. *Journal of Mathematical Chemistry*, **2000**, 27, 35-41	2.1	2
97	Molecular Quantum Similarity in QSAR and Drug Design. *Lecture Notes in Quantum Chemistry II*, **2000**,	0.6	52
96	Modeling antimalarial activity: application of Kinetic Energy Density Quantum Similarity Measures as descriptors in QSAR. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1400-7		37
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