Ramon Carb-Dorca i Carr

List of Publications by Citations

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	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	2.1	551
281	Critical analysis and extension of the Hirshfeld atoms in molecules. *Journal of Chemical Physics*, **2007**, 126, 144111	3.9	484
280	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
279	Critical thoughts on computing atom condensed Fukui functions. *Journal of Chemical Physics*, **2007**, 127, 034102	3.9	128
278	Molecular quantum similarity measures and N-dimensional representation of quantum objects. I. Theoretical foundations. *International Journal of Quantum Chemistry*, **1992**, 42, 1681-1693	2.1	108
277	Quantum similarity measures under atomic shell approximation: First order density fitting using elementary Jacobi rotations. *Journal of Computational Chemistry*, **1997**, 18, 2023-2039	3.5	100
276	Negative Fukui functions: New insights based on electronegativity equalization. *Journal of Chemical Physics*, **2003**, 118, 4349-4356	3.9	99
275	A general survey of molecular quantum similarity. *Computational and Theoretical Chemistry*, **1998**, 451, 11-23		87
274	Atomic Shell Approximation: Electron Density Fitting Algorithm Restricting Coefficients to Positive Values. *Journal of Chemical Information and Computer Sciences*, **1995**, 35, 1046-1053		85
273	Toward a global maximization of the molecular similarity function: Superposition of two molecules. *Journal of Computational Chemistry*, **1997**, 18, 826-846	3.5	84
272	Three-dimensional quantitative structure-activity relationships from tuned molecular quantum similarity measures: prediction of the corticosteroid-binding globulin binding affinity for a steroid family. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 333-44		82
271	Six questions on topology in theoretical chemistry. *Computational and Theoretical Chemistry*, **2015**, 1053, 2-16	2	81
270	Molecular quantum similarity and the fundamentals of QSAR. *Accounts of Chemical Research*, **2002**, 35, 289-95	24.3	78
269	Molecular Quantum Similarity: theoretical Framework, Ordering Principles, and Visualization Techniques. *Advances in Quantum Chemistry*, **1994**, 253-313	1.4	73
268	Modeling the structure-property relationships of nanoneedles: A journey toward nanomedicine. *Journal of Computational Chemistry*, **2009**, 30, 275-84	3.5	71
267	Nine questions on energy decomposition analysis. *Journal of Computational Chemistry*, **2019**, 40, 2248-2283	3.5	70
266	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	3.5	65

265	Molsimil - 88: Molecular similarity calculations using a CNDO-like approximation. *Computer Physics Communications*, **1989**, 55, 117-126	4.2	60
264	Molecular quantum similarity measures and N-dimensional representation of quantum objects. II. Practical applications. *International Journal of Quantum Chemistry*, **1992**, 42, 1695-1709	2.1	59
263	TGSA: A molecular superposition program based on topo-geometrical considerations. *Journal of Computational Chemistry*, **2001**, 22, 255-263	3.5	58
262	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	2.1	58
261	Quantum Mechanical Basis for Mulliken Population Analysis. *Journal of Mathematical Chemistry*, **2004**, 36, 231-239	2.1	55
260	A Mathematical Discussion on Density and Shape Functions, Vector Semispaces and Related Questions. *Journal of Mathematical Chemistry*, **2004**, 36, 191-200	2.1	54
259	Structure-Activity Relationships of a Steroid Family using Quantum Similarity Measures and Topological Quantum Similarity Indices. *QSAR and Combinatorial Science*, **1997**, 16, 465-472		52
258	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
257	Quantum mechanical origin of QSAR: theory and applications. *Computational and Theoretical Chemistry*, **2000**, 504, 181-228		52
256	Molecular Quantum Similarity in QSAR and Drug Design. *Lecture Notes in Quantum Chemistry II*, **2000**,	0.6	52
255	Molecular basis of quantitative structure-properties relationships (QSPR): a quantum similarity approach. *Journal of Computer-Aided Molecular Design*, **1999**, 13, 259-70	4.2	51
254	On quantum molecular similarity measures (QMSM) and indices (QMSI). *Journal of Mathematical Chemistry*, **1996**, 19, 47-56	2.1	51
253	Molecular electronic density fitting using elementary Jacobi rotations under atomic shell approximation. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 1188-98		50
252	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	2.1	49
251	Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. *Structural Chemistry*, **2018**, 29, 33-38	1.8	47
250	Quantum similarity measures, molecular cloud description, and structure-properties relationships. *Journal of Chemical Information and Computer Sciences*, **1992**, 32, 600-606		47
249	Application of Molecular Quantum Similarity to QSAR. *QSAR and Combinatorial Science*, **1997**, 16, 25-32		46
248	Aromaticity in linear polyacenes: generalized population analysis and molecular quantum similarity approach. *Journal of Computational Chemistry*, **2007**, 28, 152-60	3.5	46

247	Inward matrix products: extensions and applications to quantum mechanical foundations of QSAR. *Computational and Theoretical Chemistry*, **2001**, 537, 41-54		46
246	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
245	Molecular quantum similarity measures tuned 3D QSAR: an antitumoral family validation study. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 624-31		44
244	On the calculation of ab initio quantum molecular similarities for large systems: Fitting the electron density. *Journal of Computational Chemistry*, **1994**, 15, 1113-1120	3.5	44
243	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	3.9	43
242	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	16.4	43
241	Triple density molecular quantum similarity measures: A general connection between theoretical calculations and experimental results. *Molecular Engineering*, **1992**, 2, 43-64		43
240	Communications on quantum similarity, part 3: a geometric-quantum similarity molecular superposition algorithm. *Journal of Computational Chemistry*, **2011**, 32, 582-99	3.5	41
239	Molecular quantum similarity measures as an alternative to log P values in QSAR studies. *Journal of Computational Chemistry*, **1998**, 19, 1575-1583	3.5	40
238	Commentaries on quantum similarity (1): Density gradient quantum similarity. *Journal of Computational Chemistry*, **2010**, 31, 2195-212	3.5	39
237	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
236	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
235	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
234	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
233	Definition, mathematical examples and quantum chemical applications of nested summation symbols and logical Kronecker deltas. *Computers & Chemistry*, **1994**, 18, 117-126		38
232	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
231	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
230	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

229	Molecular quantum similarity analysis of estrogenic activity. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1166-76		36
228	Simple linear QSAR models based on quantum similarity measures. *Journal of Medicinal Chemistry*, **1999**, 42, 5169-80	8.3	36
227	Identification of active molecular sites using quantum-self-similarity measures. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 978-91		35
226	Quantum similarity approach to LFER: substituent and solvent effects on the acidities of carboxylic acids. *Journal of Physical Organic Chemistry*, **1999**, 12, 447-454	2.1	35
225	Tagged sets, convex sets and quantum similarity measures. *Journal of Mathematical Chemistry*, **1998**, 23, 353-364	2.1	34
224	Maximal probability domains in linear molecules. *Journal of Computational Chemistry*, **2005**, 26, 455-60	3.5	33
223	Elementary Unitary MO Transformations and SCF Theory. *Advances in Quantum Chemistry*, **1982**, 15, 215-265	2.1	33
222	Some remarks about a generalized SCF coupling operator open shell theory. *Chemical Physics Letters*, **1975**, 30, 43-48	2.5	33
221	Structure-activity relationships of phenethylamine. a comparison of quantum mechanical SCF "Ab initio" and semiempirical calculations. *Journal of the American Chemical Society*, **1975**, 97, 1338-47	16.4	33
220	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		31
219	Fuzzy sets and Boolean tagged sets. *Journal of Mathematical Chemistry*, **1997**, 22, 143-147	2.1	30
218	Modelling Toxicity using Molecular Quantum Similarity Measures. *QSAR and Combinatorial Science*, **2006**, 25, 579-589		30
217	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
216	A General Procedure to Obtain Quantum Mechanical Charge and Bond Order Molecular Parameters. *Journal of Mathematical Chemistry*, **2004**, 36, 201-210	2.1	29
215	Quantum molecular similarity measures and the n-dimensional representation of a molecular set: phenyldimethylthiazines. *Computational and Theoretical Chemistry*, **1992**, 254, 517-531		29
214	Nested summation symbols and perturbation theory. *Journal of Mathematical Chemistry*, **1993**, 13, 331-342	2.1	29
213	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
212	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

211	A Formal Comparison between Molecular Quantum Similarity Measures and Indices. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 469-475		28
210	Aromatic Compounds Aquatic Toxicity QSAR Using Molecular Quantum Similarity Measures. *SAR and QSAR in Environmental Research*, **1999**, 10, 401-422	3.5	28
209	Fast calculation of quantum chemical molecular descriptors from the electronegativity equalization method. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 422-8		27
208	General trends in atomic and nuclear quantum similarity measures. *International Journal of Quantum Chemistry*, **2000**, 77, 685-692	2.1	27
207	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
206	Molecular quantum similarity matrix based clustering of molecules using dendrograms. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 170-7		26
205	Structure-toxicity relationships of polycyclic aromatic hydrocarbons using molecular quantum similarity. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 67-80	4.2	26
204	Unconditional convergence in SCF theory: a general level shift technique. *Chemical Physics Letters*, **1977**, 47, 581-583	2.5	26
203	A comparative study of isodensity surfaces using ab initio and ASA density functions. *Journal of Molecular Graphics and Modelling*, **1998**, 16, 190-6	2.8	25
202	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
201	Molecular quantum similarity using conceptual DFT descriptors. *Journal of Chemical Sciences*, **2005**, 117, 425-435	1.8	25
200	Analysis of the changes on the potential energy surface of Menshutkin reactions induced by external perturbations. *Computational and Theoretical Chemistry*, **1996**, 371, 171-183		25
199	Quantum molecular similarity measures. *Advances in Molecular Similarity*, **1996**, 1-42		24
198	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
197	Quantum similarity and discrete representation of molecular sets. *Journal of Mathematical Chemistry*, **2011**, 49, 1558-1572	2.1	23
196	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
195	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
194	Quantum molecular similarity measures (QMSM) and the atomic shell approximation (ASA). *Advances in Molecular Similarity*, **1996**, 187-211		23

193	Quantum polyhedra, definitions, statistics and the construction of a collective quantum similarity index. *Journal of Mathematical Chemistry*, **2015**, 53, 171-182	2.1	22
192	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
191	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
190	On the statistical interpretation of density functions: Atomic shell approximation, convex sets, discrete quantum chemical molecular representations, diagonal vector spaces and related problems. *Journal of Mathematical Chemistry*, **1998**, 23, 365-375	2.1	22
189	Ab Initio Quantum Molecular Similarity Measures on Metal-Substituted Carbonic Anhydrase (MIICA, M = Be, Mg, Mn, Co, Ni, Cu, Zn, and Cd). *Journal of Chemical Information and Computer Sciences*, **1994**, 34, 1047-1053		22
188	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
187	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
186	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
185	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
184	N-dimensional Boolean hypercubes and the goldbach conjecture. *Journal of Mathematical Chemistry*, **2016**, 54, 1213-1220	2.1	21
183	Select-divide-and-conquer method for large-scale configuration interaction. *Journal of Chemical Physics*, **2006**, 125, 014108	3.9	20
182	Estimation of infinite dilution activity coefficients of organic compounds in water with neural classifiers. *AICHE Journal*, **2004**, 50, 1315-1343	3.6	20
181	Modeling large macromolecular structures using promolecular densities. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 847-52		20
180	Quantification of the influence of single-point mutations on haloalkane dehalogenase activity: a molecular quantum similarity study. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 839-46		20
179	Analyzing the Triple Density Molecular Quantum Similarity Measures with the INDSCAL Model. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 620-623		20
178	Using molecular quantum similarity measures as descriptors in quantitative structure-toxicity relationships. *SAR and QSAR in Environmental Research*, **1999**, 10, 545-56	3.5	20
177	Quantum Molecular Similarity: Theory and Applications to the Evaluation of Molecular Properties, Biological Activities and Toxicity. *Mathematical and Computational Chemistry*, **2001**, 187-320		20
176	Multimolecular polyhedra and QSPR. *Journal of Mathematical Chemistry*, **2014**, 52, 1848-1856	2.1	19

175	Molecular quantum similarity measures in Minkowski metric vector semispaces. *Journal of Mathematical Chemistry*, **2008**, 44, 628-636	2.1	19
174	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
173	Solutions to the Quantum QSPR problem in molecular spaces. *Theoretical Chemistry Accounts*, **2007**, 118, 673-679	1.9	18
172	Algebraic relationships between conceptual DFT quantities and the electronegativity equalization hardness matrix. *Chemical Physics Letters*, **2002**, 364, 357-362	2.5	18
171	Rational modelling of the voltage-dependent K+ channel inactivation by aminopyridines. *Biophysical Chemistry*, **2003**, 104, 417-27	3.5	18
170	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
169	DNA, unnatural base pairs and hypercubes. *Journal of Mathematical Chemistry*, **2018**, 56, 1353-1356	2.1	17
168	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
167	A new insight on the quantum quantitative structure-properties relationships. *International Journal of Quantum Chemistry*, **2008**, 108, 1721-1734	2.1	17
166	Similarity approach to QSAR. Application to antimycobacterial benzoxazines. *International Journal of Pharmaceutics*, **2004**, 269, 51-60	6.5	17
165	Inward matrix products, generalised density functions and Rayleigh-Schrödinger perturbation theory. *Computational and Theoretical Chemistry*, **2000**, 501-502, 173-176		17
164	Many Center AO Integral Evaluation Using Cartesian Exponential Type Orbitals (CETO'S). *Advances in Quantum Chemistry*, **1992**, 115-237	1.4	17
163	All valence electron wavefunctions and electrostatic molecular potentials under zero differential overlap approximation. *Chemical Physics Letters*, **1974**, 25, 89-91	2.5	17
162	About Erdős discrepancy conjecture. *Journal of Mathematical Chemistry*, **2016**, 54, 657-660	2.1	16
161	Collective Euclidian distances and quantum similarity. *Journal of Mathematical Chemistry*, **2013**, 51, 338-353	2.1	16
160	Scaled Euclidian distances: a general dissimilarity index with a suitably defined geometrical foundation. *Journal of Mathematical Chemistry*, **2012**, 50, 734-740	2.1	16
159	On the extension of quantum similarity to atomic nuclei: Nuclear quantum similarity. *Journal of Mathematical Chemistry*, **1998**, 23, 327-351	2.1	16
158	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

157	Structure□property relationships and momentum space quantities: Hammett □onstants. *Molecular Physics*, **2003**, 101, 3159-3162	1.7	16
156	Open Shell SCF Theory: An ab Initio Study of Some Interstellar Molecules. *Advances in Quantum Chemistry*, **1980**, 12, 159-187	1.4	16
155	Empirical quantum chemical approach to structure-gas chromatographic retention index relationship. I. Sterol acetates. *Journal of Chromatography A*, **1975**, 108, 337-44	4.5	16
154	A general multiconfiguration paired excitation self-consistent field theory (MC PE SCF). *Chemical Physics Letters*, **1977**, 47, 85-91	2.5	16
153	Divagations about the periodic table: Boolean hypercube and quantum similarity connections. *Journal of Computational Chemistry*, **2019**, 40, 2653-2663	3.5	15
152	Definition of norm coherent generalized scalar products and quantum similarity. *Journal of Mathematical Chemistry*, **2010**, 47, 331-344	2.1	15
151	Unrevealed structural requirements for auxin-like molecules by theoretical and experimental evidences. *Phytochemistry*, **2007**, 68, 237-50	4	15
150	Applications of inward matrix products and matrix wave functions to H□kel MO theory, Slater extended wave functions, spin extended functions, and Hartree method. *International Journal of Quantum Chemistry*, **2003**, 91, 607-617	2.1	15
149	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
148	Facet diagrams for quantum similarity data. *Journal of Computer-Aided Molecular Design*, **1999**, 13, 597-610	4.1	15
147	Quantum similarity matrices column set as holograms of DF molecular point clouds. *Journal of Mathematical Chemistry*, **2012**, 50, 2339-2341	2.1	14
146	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
145	The perturbation theory for non-degenerate states and the extended H□kel method. *Theoretica Chimica Acta*, **1970**, 17, 74-80		14
144	An isometric representation problem in quantum multimolecular polyhedra and similarity. *Journal of Mathematical Chemistry*, **2015**, 53, 1750-1758	2.1	13
143	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
142	Quantum similarity, volume functions and generalized Carb□ndices. *Journal of Mathematical Chemistry*, **2011**, 49, 2109-2115	2.1	13
141	A quantum similarity matrix (QSM) Aufbau procedure. *Journal of Mathematical Chemistry*, **2008**, 44, 228-234	2.1	13
140	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

139	Non-linear Terms & Variational Approach in Quantum QSPR. *Journal of Mathematical Chemistry*, **2004**, 36, 241-260	2.1	13
138	Molecular quantum similarity-based QSARs for binding affinities of several steroid sets. *Journal of Chemical Information and Computer Sciences*, **2002**, 42, 1185-93		13
137	Electrostatic molecular potential as a static index in the study of aromatic substitutions. *Chemical Physics Letters*, **1975**, 31, 267-270	2.5	13
136	Quantum similarity. *Advances in Molecular Similarity*, **1999**, 1-42		13
135	A study on Goldbach conjecture. *Journal of Mathematical Chemistry*, **2016**, 54, 1798-1809	2.1	12
134	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
133	Extended density functions. *Advances in Quantum Chemistry*, **2000**, 38, 1-63	1.4	12
132	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
131	Quantum QSAR and the eigensystems of stochastic quantum similarity matrices. *Journal of Mathematical Chemistry*, **2000**, 27, 357-376	2.1	12
130	Chemical bonds from the condition of minimal pair fluctuation: Correlated case. *International Journal of Quantum Chemistry*, **1999**, 72, 85-91	2.1	12
129	Electrostatic corrections to extended H□kel theory. *International Journal of Quantum Chemistry*, **1977**, 11, 271-276	2.1	12
128	Toward a universal quantum QSPR operator. *International Journal of Quantum Chemistry*, **2018**, 118, e25602	2.1	11
127	The general Gaussian product theorem. *Journal of Mathematical Chemistry*, **2011**, 49, 1769-1784	2.1	11
126	Mathematical Elements of Quantum Electronic Density Functions. *Advances in Quantum Chemistry*, **2005**, 121-207	1.4	11
125	A naive look on the Hohenberg□Kohn theorem. *Journal of Mathematical Chemistry*, **1999**, 25, 253-257	2.1	11
124	Extending molecular similarity to energy surfaces: Boltzmann similarity measures and indices. *Journal of Mathematical Chemistry*, **1996**, 20, 247-261	2.1	11
123	Generalized Rayleigh-Schr□dinger perturbation theory in matrix form. *Journal of Mathematical Chemistry*, **1994**, 15, 397-406	2.1	11
122	A concurrent algorithm for parallel calculation of eigenvalues and eigenvectors of real symmetric matrices. *Journal of Computational Chemistry*, **1992**, 13, 155-159	3.5	11

121	Boolean Hypercubes as time representation holders. *Journal of Mathematical Chemistry*, **2018**, 56, 1349-1352	2.1	10
120	EMP as a similarity measure: a geometric point of view. *Journal of Mathematical Chemistry*, **2013**, 51, 382-389	2.1	10
119	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
118	Smooth function topological structure descriptors based on graph-spectra. *Journal of Mathematical Chemistry*, **2008**, 44, 373-378	2.1	10
117	Jacobi Rotations: A General Procedure for Electronic Energy Optimization. *Advances in Quantum Chemistry*, **1989**, 20, 375-441	1.4	10
116	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	4.2	10
115	Aromaticity, quantum multimolecular polyhedra, and quantum QSPR fundamental equation. *Journal of Computational Chemistry*, **2016**, 37, 78-82	3.5	10
114	Refinement of a generalized Fermat's last theorem conjecture in natural vector spaces. *Journal of Mathematical Chemistry*, **2017**, 55, 1869-1877	2.1	9
113	Geometry of n-dimensional Euclidean space Gaussian enfoldments. *Journal of Mathematical Chemistry*, **2011**, 49, 2244-2249	2.1	9
112	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
111	Classification of reaction pathways via momentum-space and quantum molecular similarity measures. *Chemical Physics Letters*, **2003**, 367, 207-213	2.5	9
110	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
109	Interstellar chemistry. *Journal of Chemical Education*, **1985**, 62, 832	2.4	9
108	Ground and first excited states electrostatic molecular potentials of ketene and diazomethane. *Chemical Physics Letters*, **1974**, 28, 422-426	2.5	9
107	Quantum polyhedra in LCAO MO theory. *Molecular Physics*, **2016**, 114, 1236-1249	1.7	8
106	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
105	Least squares estimation of unknown molecular properties and quantum QSPR fundamental equation. *Journal of Mathematical Chemistry*, **2015**, 53, 1651-1656	2.1	8
104	Variational principle, Hohenberg-Kohn theorem, and density function origin shifts. *Journal of Mathematical Chemistry*, **2013**, 51, 1397-1409	2.1	8

103	Diagonal coefficient representation of density functions and quantum similarity measures. *Journal of Mathematical Chemistry*, **2008**, 44, 621-627	2.1	8
102	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
101	SCF Theory of multiplet states. *International Journal of Quantum Chemistry*, **1980**, 17, 725-736	2.1	8
100	Average fock operators. *International Journal of Quantum Chemistry*, **1980**, 18, 1207-1221	2.1	8
99	Time vectors and particle swarms defined as polyhedra in spherically enfolded spaces. *Journal of Mathematical Chemistry*, **2016**, 54, 1751-1757	2.1	7
98	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
97	On the nature of atomic shell approximation (ASA) electrostatic molecular potentials (EMP). *Journal of Mathematical Chemistry*, **2012**, 50, 981-988	2.1	7
96	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
95	n-Dimensional Euclidean space Gaussian enfoldment. *Journal of Mathematical Chemistry*, **2011**, 49, 2231-2243	2.1	7
94	An iterative method to solve the algebraic eigenvalue problem. *Journal of Mathematical Chemistry*, **1997**, 21, 395-412	2.1	7
93	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
92	Generation of Molecular Fields, Quantum Similarity Measures and Related Questions. *Journal of Mathematical Chemistry*, **2006**, 39, 495-510	2.1	7
91	Energy variation and elementary Jacobi rotations. *Computational and Theoretical Chemistry*, **1983**, 93, 15-33		7
90	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
89	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
88	Softened electrostatic molecular potentials. *Journal of Molecular Graphics and Modelling*, **2013**, 39, 39-49	2.8	6
87	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
86	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

85	Riemannian three dimensional molecular spaces. *Journal of Mathematical Chemistry*, **2008**, 44, 286-300	2.1	6
84	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
83	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
82	Molecular Nuclear Fields: A Na□e Perspective. *Journal of Mathematical Chemistry*, **2005**, 38, 671-676	2.1	6
81	DENSITY FUNCTIONS AND GENERATING WAVE FUNCTIONS **2002**, 401-412		6
80	A new look on SCF theory. *Chemical Physics Letters*, **1975**, 33, 545-549	2.5	6
79	Empirical quantum chemical approach to structure-gas chromatographic retention index relationships. *Journal of Chromatography A*, **1976**, 117, 105-116	4.5	6
78	Sequence of energy levels in molecular calculations with a nonorthogonal basis **1969**, 59, 204-217		6
77	Eigenspace manipulation in SCF theory. *International Journal of Quantum Chemistry*, **1972**, 6, 843-847	2.1	6
76	Boolean hypercubes and the structure of vector spaces. *Journal of Mathematical Sciences and Modelling*, **2018**, 1, 1-14	3	6
75	A theorem on the Gram matrix of a polyhedron. *Journal of Mathematical Chemistry*, **2017**, 55, 79-97	2.1	5
74	Enfolded conformational spaces: definition of the chemical quantum mechanical multiverse under Born□ppenheimer approximation. *Journal of Mathematical Chemistry*, **2013**, 51, 1092-1098	2.1	5
73	Position-momentum Heisenberg uncertainty in Gaussian enfoldments of Euclidian space. *Journal of Mathematical Chemistry*, **2013**, 51, 420-426	2.1	5
72	Heisenberg□ Relations in Discrete N-Dimensional Parameterized Metric Vector Spaces. *Journal of Mathematical Chemistry*, **2004**, 36, 41-54	2.1	5
71	Geometric and electronic similarities between transition structures for electrocyclizations and sigmatropic hydrogen shifts. *Theoretical Chemistry Accounts*, **2005**, 113, 205-211	1.9	5
70	Molecular Quantum Similarity Measures as Descriptors for Quantum QSAR. *Polycyclic Aromatic Compounds*, **2001**, 19, 51-71	1.3	5
69	Rayleigh-Schr□inger Perturbation Theory in Matrix Form. *Journal of Chemical Education*, **1998**, 75, 502	2.4	5
68	Multiconfigurational calculations using Elementary Jacobi Rotations. *Computational and Theoretical Chemistry*, **1985**, 120, 357-363		5

67	Comparative borazarobenzenes calculations following different methods. *Theoretica Chimica Acta*, **1969**, 14, 147-162		5
66	Conformational analysis from the viewpoint of molecular similarity. *Advances in Molecular Similarity* , **1996**, 135-165		5
65	Transformation of boolean hypercube vertices into unit interval elements: QSPR workout consequences. *Journal of Mathematical Chemistry*, **2019**, 57, 694-696	2.1	5
64	Fuzzy Hypercubes and their time-like evolution. *Journal of Mathematical Chemistry*, **2020**, 58, 1337-1344	2.1	4
63	On density function coordinate matrix. *Journal of Mathematical Chemistry*, **2013**, 51, 1681-1683	2.1	4
62	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
61	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
60	Generalized one-electron spin functions and self-similarity measures. *Journal of Mathematical Chemistry*, **2001**, 29, 41-45	2.1	4
59	Multicentric expansions for isosceles H++3 configurations. *Journal of Chemical Physics*, **1975**, 62, 2637-2639	2.1	4
58	Mathematical basis of approximate MO theories: Origin of mulliken's magic formula. *International Journal of Quantum Chemistry*, **1978**, 14, 209-212	2.1	4
57	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
56	Generalized scalar products in Minkowski metric spaces. *Journal of Mathematical Chemistry*, **2021**, 59, 1029-1045	2.1	4
55	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
54	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
53	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
52	Fermi accelerator: A new insight from quantum theory of motion. *International Journal of Quantum Chemistry*, **2015**, 115, 1733-1738	2.1	3
51	Completely soft molecular electrostatic potentials (CoSMEP) and total density functions. *Journal of Mathematical Chemistry*, **2013**, 51, 1772-1783	2.1	3
50	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

49	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
48	Comment on "Chemoselectives in acetalization, thioacetalization, oxathioacetalization and azathioacetalization". *Journal of Physical Chemistry A*, **2007**, 111, 2640	2.8	3
47	On Einstein□Podolsky□Rosen Paradox. *Journal of Mathematical Chemistry*, **2007**, 41, 209-215	2.1	3
46	Extended Sobolev and Hilbert spaces and approximate stationary solutions for electronic systems within the non-linear Schr□inger equation **2001**, 29, 3-20		3
45	A procedure to obtain an accurate approximation to a full CI wavefunction. *Journal of Mathematical Chemistry*, **1996**, 20, 263-271	2.1	3
44	A modified Del Re method. *Theoretica Chimica Acta*, **1970**, 18, 170-173		3
43	Molecular Quantum Similarity **2009**,		3
42	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
41	A study on the centroid vector of a polyhedron. *Journal of Mathematical Chemistry*, **2016**, 54, 61-71	2.1	2
40	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
39	Function extended spaces. *Journal of Mathematical Chemistry*, **2013**, 51, 660-671	2.1	2
38	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
37	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
36	The relationship between the eigenvalues and eigenvectors of a similarity matrix and its associated Carb□ndex matrix. *Journal of Mathematical Chemistry*, **2011**, 49, 6-11	2.1	2
35	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
34	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
33	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
32	Quantum chemistry, Sobolev spaces and SCF. *Journal of Mathematical Chemistry*, **2000**, 28, 59-70	2.1	2

31	A discussion on an apparent MO theory paradox. *Journal of Mathematical Chemistry*, **2000**, 27, 35-41	2.1	2
30	Note on a Roothaan procedure. *Chemical Physics Letters*, **1971**, 8, 75-76	2.5	2
29	Boolean Hypercubes, Mersenne Numbers, and the Collatz Conjecture. *Journal of Mathematical Sciences and Modelling*,120-129	3	2
28	Extended Minkowski spaces, zero norms, and Minkowski hypersurfaces. *Journal of Mathematical Chemistry*, **2021**, 59, 1875-1879	2.1	2
27	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
26	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
25	An isometric representation problem in quantum multimolecular polyhedra and similarity: (2) synisometry. *Journal of Mathematical Chemistry*, **2015**, 53, 1876-1884	2.1	1
24	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
23	Theoretical and computational aspects of extended wave functions. *International Journal of Quantum Chemistry*, **2001**, 84, 331-337	2.1	1
22	Theoretical interstellar and prebiotic organic chemistry: a tentative methodology. *Origins of Life and Evolution of Biospheres*, **1976**, 7, 163-73		1
21	Virtual orbitals in SCF theory. III: Perturbational treatment. *Chemical Physics Letters*, **1972**, 13, 82-84	2.5	1
20	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
19	The Collatz conjecture and the quantum mechanical harmonic oscillator. *Journal of Mathematical Chemistry*,1	2.1	1
18	Quantum self-similarity measures as QSAR descriptors. *Lecture Notes in Quantum Chemistry II*, **2000**, 67-836		1
17	Application of Quantum Similarity to QSAR. *Lecture Notes in Quantum Chemistry II*, **2000**, 26-38	0.6	1
16	Statistical-like signature of molecular basis sets. *Journal of Molecular Modeling*, **2018**, 24, 256	2	1
15	A naïve HMO study of the casimir effect. *Journal of Mathematical Chemistry*, **2022**, 60, 581	2.1	0
14	Shadows–hypercube, vector spaces, and non-linear optimization of QSPR procedures. *Journal of Mathematical Chemistry*,1	2.1	0

13	Determination of unknown molecular properties in molecular spaces. *Journal of Mathematical Chemistry*, **2022**, 60, 353	2.1	0
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	2.1	0
11	Analysis of solutions of time-dependent Schrödinger equation of a particle trapped in a spherical box. *Journal of Mathematical Chemistry*,1	2.1	0
10	Vector spaces defined over the unit interval. *Journal of Mathematical Chemistry*, **2019**, 57, 691-693	2.1	
9	Thermal scaling of electronic energy expressions. *Journal of Mathematical Chemistry*, **2018**, 56, 979-981	2.1	
8	Atomic thermal voltage population distributions. *Journal of Mathematical Chemistry*, **2018**, 56, 1357-1359	2.1	
7	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	
6	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	
5	Discussion on the variable Wolfsberg–Helmholtz parameter, a new simplified Löwdin transformation and the characteristic structure of the transformed EHT Hamiltonian matrices. *International Journal of Quantum Chemistry*, **2004**, 98, 26-32	2.1	
4	Quantum objects, density functions and molecular quantum similarity measures. *Lecture Notes in Quantum Chemistry II*, **2000**, 6-25	0.6	
3	Full molecular quantum similarity matrices as QSAR descriptors. *Lecture Notes in Quantum Chemistry II*, **2000**, 39-66	0.6	
2	Extension of Fermat's last theorem in Minkowski natural spaces. *Journal of Mathematical Chemistry*, **2021**, 59, 1851-1863	2.1	
1	About the construction of probability hypercubes. *Journal of Mathematical Chemistry*, **2021**, 59, 1151-1154	2.1	