Emili Besalu

List of Publications by Year
in descending order

72 papers	1,653 citations	318942 23 h-index	355658 38 g-index
72 all docs	72 docs citations	72 times ranked	1281 citing authors

#	Article	IF	Citations
1	Free-Radical Photopolymerization for Curing Products for Refinish Coatings Market. Polymers, 2022, 14, 2856.	2.0	34
2	Ranking Series of Cancer-Related Gene Expression Data by Means of the Superposing Significant Interaction Rules Method. Biomolecules, 2020, 10, 1293.	1.8	1
3	Investigation of Volatiles in Cork Samples Using Chromatographic Data and the Superposing Significant Interaction Rules (SSIR) Chemometric Tool. Biomolecules, 2020, 10, 896.	1.8	3
4	Modeling Binary Fingerprint Descriptors With the Superposing Significant Interaction Rules (SSIR) Method. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 98-107.	1.1	0
5	Checking the Efficacy of Two Basic Descriptors With a Set of Properties of Alkanes. International Journal of Quantitative Structure-Property Relationships, 2019, 4, 67-87.	1.1	0
6	Modeling Properties with Artificial Neural Networks and Multilinear Least-Squares Regression: Advantages and Drawbacks of the Two Methods. Applied Sciences (Switzerland), 2018, 8, 1094.	1.3	8
7	Tryptophan-Containing Cyclic Decapeptides with Activity against Plant Pathogenic Bacteria. Molecules, 2017, 22, 1817.	1.7	7
8	Molecular Rearrangement of an Aza-Scorpiand Macrocycle Induced by pH: A Computational Study. International Journal of Molecular Sciences, 2016, 17, 1131.	1.8	6
9	Fast Modeling of Binding Affinities by Means of Superposing Significant Interaction Rules (SSIR) Method. International Journal of Molecular Sciences, 2016, 17, 827.	1.8	7
10	Discriminating Drug-Like Compounds by Partition Trees with Quantum Similarity Indices and Graph Invariants. Current Pharmaceutical Design, 2016, 22, 5179-5195.	0.9	3
11	Superposing Significant Interaction Rules (SSIR) Method: A simple Procedure for Rapid Ranking of Congeneric Compounds. Croatica Chemica Acta, 2016, 89, .	0.1	3
12	Monitoring of sixteen fragrance allergens and two polycyclic musks in wastewater treatment plants by solid phase microextraction coupled to gas chromatography. Chemosphere, 2015, 119, 363-370.	4.2	52
13	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
14	Sequential discriminant classification of environments with different levels of exposure to tobacco smoke. Science of the Total Environment, 2014, 490, 899-904.	3.9	2
15	A Probabilistic Analysis About the Concepts of Difficulty and Usefulness of a Molecular Ranking Classification. Current Computer-Aided Drug Design, 2014, 10, 107-114.	0.8	1
16	EMP as a similarity measure: a geometric point of view. Journal of Mathematical Chemistry, 2013, 51, 382-389.	0.7	13
17	Function extended spaces. Journal of Mathematical Chemistry, 2013, 51, 660-671.	0.7	3
18	From Periodic Properties to a Periodic Table Arrangement. Journal of Chemical Education, 2013, 90, 1009-1013.	1.1	7

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19	Completely soft molecular electrostatic potentials (CoSMEP) and total density functions. Journal of Mathematical Chemistry, 2013, 51, 1772-1783.	0.7	4
20	The connection between inverse and classical calibration. Talanta, 2013, 116, 45-49.	2.9	10
21	Softened electrostatic molecular potentials. Journal of Molecular Graphics and Modelling, 2013, 39, 39-49.	1.3	7
22	A headspace needle-trap method for the analysis of volatile organic compounds in whole blood. Journal of Chromatography A, 2012, 1252, 23-30.	1.8	35
23	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
24	On the nature of atomic shell approximation (ASA) electrostatic molecular potentials (EMP). Journal of Mathematical Chemistry, 2012, 50, 981-988.	0.7	10
25	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
26	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
27	The general Gaussian product theorem. Journal of Mathematical Chemistry, 2011, 49, 1769-1784.	0.7	15
28	Geometry of n-dimensional Euclidean space Gaussian enfoldments. Journal of Mathematical Chemistry, 2011, 49, 2244-2249.	0.7	10
29	Communications on quantum similarity, part 3: A geometricâ€quantum similarity molecular superposition algorithm. Journal of Computational Chemistry, 2011, 32, 582-599.	1.5	48
30	Multivariate analysis of volatile compounds detected by headspace solid-phase microextraction/gas chromatography: A tool for sensory classification of cork stoppers. Food Chemistry, 2011, 126, 1978-1984.	4.2	18
31	Odour-causing organic compounds in wastewater treatment plants: Evaluation of headspace solid-phase microextraction as a concentration technique. Journal of Chromatography A, 2011, 1218, 4863-4868.	1.8	27
32	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
33	Two-Variable Linear Regression: Modeling with Orthogonal Least-Squares Analysis. Journal of Chemical Education, 2010, 87, 994-995.	1.1	9
34	Antimicrobial cyclic decapeptides with anticancer activity. Peptides, 2010, 31, 2017-2026.	1.2	23
35	The vibrational auto-adjusting perturbation theory. Theoretical Chemistry Accounts, 2009, 123, 41-49.	0.5	8
36	INTERNAL TEST SET (ITS) METHOD: A NEW CROSS-VALIDATION TECHNIQUE TO ASSESS THE PREDICTIVE CAPABILITY OF QSAR MODELS. APPLICATION TO A BENCHMARK SET OF STEROIDS. Journal of the Chilean Chemical Society, 2008, 53, .	0.5	6

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37	A library of linear undecapeptides with bactericidal activity against phytopathogenic bacteria. Peptides, 2007, 28, 2276-2285.	1.2	145
38	Internal Standardizationâ˜Atomic Spectrometry and Geographical Pattern Recognition Techniques for the Multielement Analysis and Classification of Catalonian Red Wines. Journal of Agricultural and Food Chemistry, 2007, 55, 219-225.	2.4	41
39	Trends and Plot Methods in MLR Studies. Journal of Chemical Information and Modeling, 2007, 47, 751-760.	2.5	21
40	Ethanol/Water Extraction Combined with Solid-Phase Extraction and Solid-Phase Microextraction Concentration for the Determination of Chlorophenols in Cork Stoppers. Journal of Agricultural and Food Chemistry, 2006, 54, 627-632.	2.4	14
41	Improvement of cyclic decapeptides against plant pathogenic bacteria using a combinatorial chemistry approach. Peptides, 2006, 27, 2575-2584.	1.2	55
42	An overlooked property of plot methods. Journal of Mathematical Chemistry, 2006, 39, 475-484.	0.7	17
43	Generation of Molecular Fields, Quantum Similarity Measures and Related Questions. Journal of Mathematical Chemistry, 2006, 39, 495-510.	0.7	9
44	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
45	Molecular Quantum Similarity and the Fundamentals of QSAR. Accounts of Chemical Research, 2002, 35, 289-295.	7.6	99
46	Identification of Active Molecular Sites Using Quantum-Self-Similarity Measures. Journal of Chemical Information and Computer Sciences, 2001, 41, 978-991.	2.8	39
47	On the quadratic reaction path evaluated in a reduced potential energy surface model and the problem to locate transition states. Journal of Computational Chemistry, 2001, 22, 387-406.	1.5	52
48	Fast Computation of Cross-Validated Properties in Full Linear Leave-Many-Out Procedures. Journal of Mathematical Chemistry, 2001, 29, 191-204.	0.7	31
49	On the optimal selection of principal components in QSPR studies. Journal of Mathematical Chemistry, 2001, 29, 21-34.	0.7	2
50	Quantum chemistry, Sobolev spaces and SCF. Journal of Mathematical Chemistry, 2000, 28, 59-70.	0.7	4
51	Virtual generation of agents against Mycobacterium tuberculosis. A QSAR study. Molecular Diversity, 2000, 6, 107-120.	2.1	10
52	A naive look on the Hohenbergâ€“Kohn theorem. Journal of Mathematical Chemistry, 1999, 25, 253-257.	0.7	13
53	Title is missing!. Journal of Mathematical Chemistry, 1999, 25, 85-92.	0.7	15
54	Remarks on large-scale matrix diagonalization using a Lagrange-Newton-Raphson minimization in a subspace. Theoretical Chemistry Accounts, 1999, 103, 163-166.	0.5	12

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55	Prediction of approximate transition states by Bell-Evans-Polanyi principle: I. Journal of Computational Chemistry, 1999, 20, 1112-1129.	1.5	28
56	Prediction of approximate transition states by Bell-Evans-Polanyi principle: II. Gas phase unimolecular decomposition of methyldioxirane. Journal of Computational Chemistry, 1999, 20, 1130-1137.	1.5	5
57	Title is missing!. Journal of Mathematical Chemistry, 1998, 22, 85-95.	0.7	6
58	A general survey of molecular quantum similarity. Computational and Theoretical Chemistry, 1998, 451, 11-23.	1.5	108
59	Calculation of clustered eigenvalues of large matrices using variance minimization method. Journal of Computational Chemistry, 1998, 19, 1777-1785.	1.5	7
60	On the automatic restricted-step rational-function-optimization method. Theoretical Chemistry Accounts, 1998, 100, 265-274.	0.5	41
61	Exploring the Rayleigh-Ritz Variational Principle. Journal of Chemical Education, 1998, 75, 105.	1.1	14
62	Molecular Quantum Similarity Measures Tuned 3D QSAR:â€‰ An Antitumoral Family Validation Study. Journal of Chemical Information and Computer Sciences, 1998, 38, 624-631.	2.8	57
63	Rayleigh-SchrÃ¶dinger Perturbation Theory in Matrix Form. Journal of Chemical Education, 1998, 75, 502.	1.1	6
64	An iterative method to solve the algebraic eigenvalue problem. Journal of Mathematical Chemistry, 1997, 21, 395-412.	0.7	7
65	Application of Molecular Quantum Similarity to QSAR. QSAR and Combinatorial Science, 1997, 16, 25-32.	1.4	58
66	Structure-Activity Relationships of a Steroid Family using Quantum Similarity Measures and Topological Quantum Similarity Indices. QSAR and Combinatorial Science, 1997, 16, 465-472.	1.4	62
67	Extending molecular similarity to energy surfaces: Boltzmann similarity measures and indices. Journal of Mathematical Chemistry, 1996, 20, 247-261.	0.7	14
68	A procedure to obtain an accurate approximation to a full CI wavefunction. Journal of Mathematical Chemistry, 1996, 20, 263-271.	0.7	5
69	Molecular Quantum Similarity: theoretical Framework, Ordering Principles, and Visualization Techniques. Advances in Quantum Chemistry, 1994, , 253-313.	0.4	89
70	Definition, mathematical examples and quantum chemical applications of nested summation symbols and logical Kronecker deltas. Computers & Chemistry, 1994, 18, 117-126.	1.2	44
71	AO integral evaluation using Cartesian exponential type orbitals (CETOs). Canadian Journal of Chemistry, 1992, 70, 353-361.	0.6	10
72	Many Center AO Integral Evaluation Using Cartesian Exponential Type Orbitals (CETO'S). Advances in Quantum Chemistry, 1992, , 115-237.	0.4	21