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List of Publications by Year
in descending order

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43 papers	2,291 citations	236925 25 h-index	276875 41 g-index
47 all docs	47 docs citations	47 times ranked	1921 citing authors

#	Article	IF	Citations
1	Assessment of 3D models for allergen research. Proteins: Structure, Function and Bioinformatics, 2013, 81, 545-554.	2.6	16
2	Chemical Graphs, Molecular Matrices and Topological Indices in Chemoinformatics and Quantitative Structure-Activity Relationships§. Current Computer-Aided Drug Design, 2013, 9, 153-163.	1.2	60
3	Flow Network QSAR for the Prediction of Physicochemical Properties by Mapping an Electrical Resistance Network onto a Chemical Reaction Poset§. Current Computer-Aided Drug Design, 2013, 9, 233-240.	1.2	0
4	AllerML: Markup language for allergens. Regulatory Toxicology and Pharmacology, 2011, 60, 151-160.	2.7	9
5	Network-QSAR with Reaction Poset Quantitative Superstructure-Activity Relationships (QSSAR) for PCB Chromatographic Properties. Current Bioinformatics, 2011, 6, 25-34.	1.5	13
6	An Allergen Portrait Gallery: Representative Structures and an Overview of IgE Binding Surfaces. Bioinformatics and Biology Insights, 2010, 4, BBI.S5737.	2.0	19
7	Structural analysis of linear and conformational epitopes of allergens. Regulatory Toxicology and Pharmacology, 2009, 54, S11-S19.	2.7	33
8	Characteristic motifs for families of allergenic proteins. Molecular Immunology, 2009, 46, 559-568.	2.2	73
9	The property distance index PD predicts peptides that cross-react with IgE antibodies. Molecular Immunology, 2009, 46, 873-883.	2.2	51
10	Meet the Guest Editor. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 520-520.	1.1	0
11	Comprehensive 3D-modeling of allergenic proteins and amino acid composition of potential conformational IgE epitopes. Molecular Immunology, 2008, 45, 3740-3747.	2.2	67
12	Weka Machine Learning for Predicting the Phospholipidosis Inducing Potential. Current Topics in Medicinal Chemistry, 2008, 8, 1691-1709.	2.1	81
13	Robust Quantitative Modeling of Peptide Binding Affinities for MHC Molecules Using Physical-Chemical Descriptors. Protein and Peptide Letters, 2007, 14, 903-916.	0.9	21
14	Applications of Support Vector Machines in Chemistry. Reviews in Computational Chemistry, 2007, , 291-400.	1.5	261
15	Four New Topological Indices Based on the Molecular Path Code. Journal of Chemical Information and Modeling, 2007, 47, 716-731.	5.4	21
16	Bioinformatics Approaches to Classifying Allergens and Predicting Cross-Reactivity. Immunology and Allergy Clinics of North America, 2007, 27, 1-27.	1.9	81
17	Posetic Cluster Expansion for Substitution-Reaction Networks and Application to Methylated Cyclobutanes. Journal of Mathematical Chemistry, 2007, 41, 355-379.	1.5	10
18	Prediction of Environmental Properties for Chlorophenols with Posetic Quantitative Super-Structure/Property Relationships (QSSPR). International Journal of Molecular Sciences, 2006, 7, 358-374.	4.1	25

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19	Modeling the bioconcentration factors and bioaccumulation factors of polychlorinated biphenyls with posetic quantitative super-structure/activity relationships (QSSAR). Molecular Diversity, 2006, 10, 133-145.	3.9	94
20	Large â€œPillowâ€•Fullerenes Hydrogenated at the Interâ€šsheet â€œSeamâ€• Fullerenes Nanotubes and Carbon Nanostructures, 2005, 13, 109-129.	2.1	1
21	Common Physicalâ^'Chemical Properties Correlate with Similar Structure of the IgE Epitopes of Peanut Allergens. Journal of Agricultural and Food Chemistry, 2005, 53, 8752-8759.	5.2	43
22	Posetic Quantitative Superstructure/Activity Relationships (QSSARs) for Chlorobenzenes. Journal of Chemical Information and Modeling, 2005, 45, 870-879.	5.4	31
23	Using Property Based Sequence Motifs and 3D Modeling to Determine Structure and Functional Regions of Proteins. Current Medicinal Chemistry, 2004, 11, 583-593.	2.4	50
24	Detecting Potential IgE-Reactive Sites on Food Proteins Using a Sequence and Structure Database, SDAP-Food. Journal of Agricultural and Food Chemistry, 2003, 51, 4830-4837.	5.2	55
25	SDAP: database and computational tools for allergenic proteins. Nucleic Acids Research, 2003, 31, 359-362.	14.5	246
26	Data mining of sequences and 3D structures of allergenic proteins. Bioinformatics, 2002, 18, 1358-1364.	4.1	87
27	Computing Wiener-Type Indices for Virtual Combinatorial Libraries Generated from Heteroatom-Containing Building Blocks. Journal of Chemical Information and Computer Sciences, 2002, 42, 8-22.	2.8	20
28	QSAR for dihydrofolate reductase inhibitors with molecular graph structural descriptors. Computational and Theoretical Chemistry, 2002, 582, 39-51.	1.5	20
29	Wiener Index Extension by Counting Even/Odd Graph Distances. Journal of Chemical Information and Computer Sciences, 2001, 41, 536-549.	2.8	53
30	Quasi-orthogonal Basis Sets of Molecular Graph Descriptors as a Chemical Diversity Measure. Journal of Chemical Information and Computer Sciences, 2000, 40, 126-134.	2.8	30
31	Identification of Groupings of Graph Theoretical Molecular Descriptors Using a Hybrid Cluster Analysis Approach. Journal of Chemical Information and Computer Sciences, 2000, 40, 1128-1146.	2.8	23
32	QSAR Comparative Study of Wiener Descriptors for Weighted Molecular Graphs. Journal of Chemical Information and Computer Sciences, 2000, 40, 1412-1422.	2.8	86
33	Evaluation in Quantitative Structureâ^'Property Relationship Models of Structural Descriptors Derived from Information-Theory Operators. Journal of Chemical Information and Computer Sciences, 2000, 40, 631-643.	2.8	33
34	Comparison of Weighting Schemes for Molecular Graph Descriptors:â€‰ Application in Quantitative Structureâ^'Retention Relationship Models for Alkylphenols in Gasâ^'Liquid Chromatography. Journal of Chemical Information and Computer Sciences, 2000, 40, 732-743.	2.8	33
35	The neural network MolNet prediction of alkane enthalpies. Analytica Chimica Acta, 1999, 384, 271-284.	5.4	17
36	Quantitative structure-property relationship study of normal boiling points for halogen-/ oxygen-/ sulfur-containing organic compounds using the CODESSA program. Tetrahedron, 1998, 54, 9129-9142.	1.9	54

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37	Design of Topological Indices. Part 10. Parameters Based on Electronegativity and Covalent Radius for the Computation of Molecular Graph Descriptors for Heteroatom-Containing Molecules. Journal of Chemical Information and Computer Sciences, 1998, 38, 395-401.	2.8	69
38	Extended Wiener indices. A new set of descriptors for quantitative structure-property studies. New Journal of Chemistry, 1998, 22, 819-822.	2.8	50
39	Degeneracy of Topologic Distance Descriptors for Cubic Molecular Graphs:â€‰ Examples of Small Fullerenes. Journal of Chemical Information and Computer Sciences, 1997, 37, 485-488.	2.8	9
40	Chemical graphs with degenerate topological indices based on information on distances. Journal of Mathematical Chemistry, 1993, 14, 21-33.	1.5	24
41	Design of topological indices. Part 4. Reciprocal distance matrix, related local vertex invariants and topological indices. Journal of Mathematical Chemistry, 1993, 12, 309-318.	1.5	243
42	Computer generation of acyclic graphs based on local vertex invariants and topological indices. Derived canonical labelling and coding of trees and alkanes. Journal of Mathematical Chemistry, 1992, 11, 79-105.	1.5	34
43	Structural Database of Allergenic Proteins (SDAP). , 0, , 257-283.		6