

Johann Gasteiger

List of Publications by Year in descending order

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106
papers

13,288
citations

41258

49
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45213

90
g-index

212
all docs

212
docs citations

212
times ranked

11321
citing authors

#	ARTICLE	IF	CITATIONS
1	Chemistry in Times of Artificial Intelligence. ChemPhysChem, 2020, 21, 2233-2242.	1.0	46
2	Performance of radial distribution function-based descriptors in the chemoinformatic studies of HIV-1 protease. Future Medicinal Chemistry, 2020, 12, 299-309.	1.1	7
3	[Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Kimito Funatsu "The Driving Force of Chemoinformatics in Japan. Journal of Computer Aided Chemistry, 2019, 20, 32-34.	0.3	0
4	Leaving us with fond memories, smiles, SMILES and, alas, tears: a tribute to David Weininger, 1952"2016. Journal of Computer-Aided Molecular Design, 2018, 32, 313-319.	1.3	1
5	Chemical Reactions. , 2018, , 83-83.		0
6	Chemoinformatics: Achievements and Challenges, a Personal View. Molecules, 2016, 21, 151.	1.7	63
7	Explorations into Chemical Reactions and Biochemical Pathways. Molecular Informatics, 2016, 35, 588-592.	1.4	1
8	Classification of Mixtures of Chinese Herbal Medicines Based on a Self-organizing Map (SOM). Molecular Informatics, 2016, 35, 109-115.	1.4	22
9	New Publicly Available Chemical Query Language, CSRML, To Support Chemotype Representations for Application to Data Mining and Modeling. Journal of Chemical Information and Modeling, 2015, 55, 510-528.	2.5	183
10	Computing target complexity. Nature Chemistry, 2015, 7, 619-620.	6.6	17
11	Combining Chemoinformatics with Bioinformatics: In Silico Prediction of Bacterial Flavor-Forming Pathways by a Chemical Systems Biology Approach "Reverse Pathway Engineering". PLoS ONE, 2014, 9, e84769.	1.1	33
12	QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010.	2.9	1,401
13	Solved and Unsolved Problems of Chemoinformatics. Molecular Informatics, 2014, 33, 454-457.	1.4	8
14	Similarity Perception of Reactions Catalyzed by Oxidoreductases and Hydrolases Using Different Classification Methods. Journal of Chemical Information and Modeling, 2010, 50, 1089-1100.	2.5	18
15	Investigations of Enzyme-Catalyzed Reactions Based on Physicochemical Descriptors Applied to Hydrolases. Journal of Chemical Information and Modeling, 2009, 49, 1525-1534.	2.5	25
16	Uncovering metabolic pathways relevant to phenotypic traits of microbial genomes. Genome Biology, 2009, 10, R28.	13.9	39
17	Comparison of Multilabel and Single-Label Classification Applied to the Prediction of the Isoform Specificity of Cytochrome P450 Substrates. Journal of Chemical Information and Modeling, 2009, 49, 2588-2605.	2.5	50
18	Encoding Absolute Configurations with Chiral Enantiophore Descriptors. Application to the Order of Elution of Enantiomers in Liquid Chromatography. QSAR and Combinatorial Science, 2008, 27, 1326-1336.	1.5	17

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19	Ligand-Based Models for the Isoform Specificity of Cytochrome P450 3A4, 2D6, and 2C9 Substrates. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1688-1701.	2.5	93
20	Self-Organizing Maps for Identification of New Inhibitors of P-Glycoprotein. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 1698-1702.	2.9	55
21	Modeling chemical reactions for drug design. <i>Journal of Computer-Aided Molecular Design</i> , 2007, 21, 33-52.	1.3	11
22	Structure and reaction based evaluation of synthetic accessibility. <i>Journal of Computer-Aided Molecular Design</i> , 2007, 21, 311-325.	1.3	140
23	Of Molecules and Humans. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 6429-6434.	2.9	52
24	Prediction of pKa Values for Aliphatic Carboxylic Acids and Alcohols with Empirical Atomic Charge Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 2256-2266.	2.5	66
25	Query Generation to Search for Inhibitors of Enzymatic Reactions. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 2333-2341.	2.5	9
26	Impact of Conformational Flexibility on Three-Dimensional Similarity Searching Using Correlation Vectors. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 2324-2332.	2.5	51
27	Development of a Structural Model for NF- κ B Inhibition of Sesquiterpene Lactones Using Self-Organizing Neural Networks. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 2241-2252.	2.9	54
28	Cheminformatics: a new field with a long tradition. <i>Analytical and Bioanalytical Chemistry</i> , 2006, 384, 57-64.	1.9	65
29	Sesquiterpene lactone-based classification of three Asteraceae tribes: a study based on self-organizing neural networks applied to chemosystematics. <i>Phytochemistry</i> , 2005, 66, 345-353.	1.4	58
30	Fingal: A Novel Approach to Geometric Fingerprinting and a Comparative Study of Its Application to 3D-QSAR Modelling. <i>QSAR and Combinatorial Science</i> , 2005, 24, 480-484.	1.5	13
31	Prediction of Enantiomeric Excess in a Combinatorial Library of Catalytic Enantioselective Reactions. <i>ACS Combinatorial Science</i> , 2005, 7, 298-301.	3.3	43
32	Use of Structure Descriptors To Discriminate between Modes of Toxic Action of Phenols. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 200-208.	2.5	42
33	Comparison of Different Classification Methods Applied to a Mode of Toxic Action Data Set. <i>QSAR and Combinatorial Science</i> , 2004, 23, 779-791.	1.5	33
34	Chirality Codes and Molecular Structure. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 831-836.	2.8	37
35	A Graph-Based Genetic Algorithm and Its Application to the Multiobjective Evolution of Median Molecules. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1079-1087.	2.8	151
36	Enabling the exploration of biochemical pathways. <i>Organic and Biomolecular Chemistry</i> , 2004, 2, 3226-3237.	1.5	49

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37	Neural networks as data mining tools in drug design. <i>Journal of Physical Organic Chemistry</i> , 2003, 16, 232-245.	0.9	60
38	Prediction of Aqueous Solubility of Organic Compounds by Topological Descriptors. <i>QSAR and Combinatorial Science</i> , 2003, 22, 821-829.	1.5	57
39	Prediction of Aqueous Solubility of Organic Compounds Based on a 3D Structure Representation. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 429-434.	2.8	138
40	Physicochemical Effects in the Representation of Molecular Structures for Drug Designing. <i>Mini-Reviews in Medicinal Chemistry</i> , 2003, 3, 789-796.	1.1	17
41	Use of the Kohonen Neural Network for Rapid Screening of Ex Vivo Anti-HIV Activity of Styrylquinolines. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 4647-4654.	2.9	82
42	Prediction of enantiomeric selectivity in chromatography. <i>Journal of Molecular Graphics and Modelling</i> , 2002, 20, 373-388.	1.3	48
43	Prediction of ¹ H NMR Chemical Shifts Using Neural Networks. <i>Analytical Chemistry</i> , 2002, 74, 80-90.	3.2	178
44	New Description of Molecular Chirality and Its Application to the Prediction of the Preferred Enantiomer in Stereoselective Reactions. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 369-375.	2.8	58
45	Neural networks and genetic algorithms in drug design. <i>Drug Discovery Today</i> , 2001, 6, 102-108.	3.2	71
46	Prediction of three-dimensional molecular structures using information from infrared spectra. <i>Analytica Chimica Acta</i> , 2000, 420, 145-154.	2.6	44
47	Steroid binding by antibodies and artificial receptors: exploration of theoretical methods to determine the origins of binding affinities and specificities. <i>Journal of Computer-Aided Molecular Design</i> , 2000, 14, 611-629.	1.3	4
48	Computer-assisted synthesis and reaction planning in combinatorial chemistry. <i>Journal of Computer - Aided Molecular Design</i> , 2000, 20, 245-264.	1.0	25
49	The Search for the Spatial and Electronic Requirements of a Drug. <i>Journal of Molecular Modeling</i> , 2000, 6, 358-378.	0.8	26
50	Simulation of Organic Reactions: From the Degradation of Chemicals to Combinatorial Synthesis. <i>Journal of Chemical Information and Computer Sciences</i> , 2000, 40, 482-494.	2.8	51
51	Deriving the 3D structure of organic molecules from their infrared spectra. <i>Vibrational Spectroscopy</i> , 1999, 19, 151-164.	1.2	274
52	Superposition of Three-Dimensional Chemical Structures Allowing for Conformational Flexibility by a Hybrid Method. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 220-232.	2.8	90
53	Classification of Organic Reactions: Similarity of Reactions Based on Changes in the Electronic Features of Oxygen Atoms at the Reaction Sites ¹ . <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 210-219.	2.8	52
54	Overcoming the Limitations of a Connection Table Description: A Universal Representation of Chemical Species. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 705-714.	2.8	42

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55	Infrared Spectra Simulation of Substituted Benzene Derivatives on the Basis of a 3D Structure Representation. <i>Analytical Chemistry</i> , 1997, 69, 2398-2405.	3.2	80
56	Knowledge Discovery in Reaction Databases: A Landscaping Organic Reactions by a Self-Organizing Neural Network. <i>Journal of the American Chemical Society</i> , 1997, 119, 4033-4042.	6.6	72
57	Chemical Information in 3D Space. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 1030-1037.	2.8	176
58	Locating Biologically Active Compounds in Medium-Sized Heterogeneous Datasets by Topological Autocorrelation Vectors: % Dopamine and Benzodiazepine Agonists. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 1205-1213.	2.8	138
59	The Coding of the Three-Dimensional Structure of Molecules by Molecular Transforms and Its Application to Structure-Spectra Correlations and Studies of Biological Activity. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 334-344.	2.8	314
60	Computer-Assisted Planning of Organic Syntheses: The Second Generation of Programs. <i>Angewandte Chemie International Edition in English</i> , 1996, 34, 2613-2633.	4.4	104
61	Comparison of structurally different allosteric modulators of muscarinic receptors by self-organizing neural networks. <i>Journal of Molecular Graphics</i> , 1996, 14, 185-193.	1.7	32
62	The comparison of geometric and electronic properties of molecular surfaces by neural networks: Application to the analysis of corticosteroid-binding globulin activity of steroids. <i>Journal of Computer-Aided Molecular Design</i> , 1996, 10, 521-534.	1.3	79
63	Computergestützte Planung organischer chemischer Synthesen: die zweite Programmgeneration. <i>Angewandte Chemie</i> , 1995, 107, 2807-2829.	1.6	12
64	Autocorrelation of Molecular Surface Properties for Modeling Corticosteroid Binding Globulin and Cytosolic Ah Receptor Activity by Neural Networks. <i>Journal of the American Chemical Society</i> , 1995, 117, 7769-7775.	6.6	325
65	Computer-assisted prediction of the degradation of chemicals: hydrolysis of amides and benzoylphenylureas. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1995, , 193-204.	0.9	21
66	Classification of multicomponent analytical data of olive oils using different neural networks. <i>Analytica Chimica Acta</i> , 1994, 292, 219-234.	2.6	102
67	Hash codes for the identification and classification of molecular structure elements. <i>Journal of Computational Chemistry</i> , 1994, 15, 793-813.	1.5	88
68	Comparison of Automatic Three-Dimensional Model Builders Using 639 X-ray Structures. <i>Journal of Chemical Information and Computer Sciences</i> , 1994, 34, 1000-1008.	2.8	596
69	Representation of Molecular Electrostatic Potentials by Topological Feature Maps. <i>Journal of the American Chemical Society</i> , 1994, 116, 4608-4620.	6.6	118
70	Neural Networks in Chemistry. <i>Angewandte Chemie International Edition in English</i> , 1993, 32, 503-527.	4.4	418
71	Neuronale Netze in der Chemie. <i>Angewandte Chemie</i> , 1993, 105, 510-536.	1.6	60
72	A combined application of two different neural network types for the prediction of chemical reactivity. <i>Journal of the American Chemical Society</i> , 1993, 115, 9148-9159.	6.6	82

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73	From atoms and bonds to three-dimensional atomic coordinates: automatic model builders. <i>Chemical Reviews</i> , 1993, 93, 2567-2581.	23.0	400
74	Similarity concepts for the planning of organic reactions and syntheses. <i>Journal of Chemical Information and Computer Sciences</i> , 1992, 32, 700-712.	2.8	44
75	The generation of 3D models of host-guest complexes. <i>Analytica Chimica Acta</i> , 1992, 265, 233-241.	2.6	69
76	Automated derivation of reaction rules for the EROS 6.0 system for reaction prediction. <i>Analytica Chimica Acta</i> , 1990, 235, 163-168.	2.6	46
77	ChemInform - an integrated information system on chemical reactions. <i>Journal of Chemical Information and Computer Sciences</i> , 1990, 30, 400-402.	2.8	25
78	A quantitative description of fundamental polar reaction types. Proton- and hydride-transfer reactions connecting alcohols and carbonyl compounds in the gas phase. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1986, , 447.	0.9	10
79	Correlation analyses of the aqueous-phase acidities of alcohols and gem-diols, and of carbonyl hydration equilibria using electronic and structural parameters. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1986, , 455.	0.9	19
80	Electronegativity equalization: application and parametrization. <i>Journal of the American Chemical Society</i> , 1985, 107, 829-835.	6.6	429
81	Calculation of the Charge Distribution in Conjugated Systems by a Quantification of the Resonance Concept. <i>Angewandte Chemie International Edition in English</i> , 1985, 24, 687-689.	4.4	96
82	Quantitative models of gas-phase proton-transfer reactions involving alcohols, ethers, and their thio analogs. Correlation analyses based on residual electronegativity and effective polarizability. <i>Journal of the American Chemical Society</i> , 1984, 106, 6489-6495.	6.6	75
83	New empirical models of substituent polarizability and their application to stabilisation effects in positively charged species. <i>Tetrahedron Letters</i> , 1983, 24, 2537-2540.	0.7	34
84	Residual electronegativity - an empirical quantification of polar influences and its application to the proton affinity of amines. <i>Tetrahedron Letters</i> , 1983, 24, 2541-2544.	0.7	83
85	Prediction of proton magnetic resonance shifts: The dependence on hydrogen charges obtained by iterative partial equalization of orbital electronegativity. <i>Magnetic Resonance in Chemistry</i> , 1981, 15, 353-360.	0.7	123
86	The Principle of Minimum Chemical Distance(PMCD). <i>Angewandte Chemie International Edition in English</i> , 1980, 19, 495-505.	4.4	59
87	Iterative partial equalization of orbital electronegativity—a rapid access to atomic charges. <i>Tetrahedron</i> , 1980, 36, 3219-3228.	1.0	3,706
88	New Applications of Computers in Chemistry. <i>Angewandte Chemie International Edition in English</i> , 1979, 18, 111-123.	4.4	98
89	An Algorithm for the Perception of Synthetically Important Rings. <i>Journal of Chemical Information and Computer Sciences</i> , 1979, 19, 43-48.	2.8	52
90	A new model for calculating atomic charges in molecules. <i>Tetrahedron Letters</i> , 1978, 19, 3181-3184.	0.7	446

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91	Chlor-, Brom- und Jod-cyclooctatetraen: Darstellung und einige Reaktionen. Chemische Berichte, 1971, 104, 2412-2419.	0.2	49
92	Methods for Data Analysis. , 0, , 1079-1081.		0
93	Chemistry on the Internet. , 0, , 794-843.		4
94	The Data. , 0, , 389-391.		0
95	Descriptors for Chemical Compounds. , 0, , 977-979.		1
96	Databases/Data Sources. , 0, , 491-493.		0
97	Representation of Chemical Reactions. , 0, , 345-347.		0
98	Representation of Chemical Compounds. , 0, , 21-26.		0
99	Calculation of Physical and Chemical Data. , 0, , 917-919.		0
100	Patent Databases. , 0, , 743-755.		0
101	Bibliographic Databases. , 0, , 507-522.		0
102	Searching Chemical Structures. , 0, , 865-867.		0
103	Calculation of Structure Descriptors. , 0, , 349-396.		0
104	Modeling and Prediction of Properties (QSPR/QSAR). , 0, , 345-347.		0
105	Representation of Chemical Reactions. , 0, , 121-154.		0
106	Empirical Approaches to the Calculation of Properties. , 0, , 269-278.		0