# Johann Gasteiger

## List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/8156201/publications.pdf

Version: 2024-02-01

| | | | |
|---|---|---|---|
| 106 papers | 13,288 citations | 41258 49 h-index | 45213 90 g-index |
| 212 all docs | 212 docs citations | 212 times ranked | 11321 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Iterative partial equalization of orbital electronegativityâ€”a rapid access to atomic charges. Tetrahedron, 1980, 36, 3219-3228. | 1.0 | 3,706 |
| 2 | QSAR Modeling: Where Have You Been? Where Are You Going To?. Journal of Medicinal Chemistry, 2014, 57, 4977-5010. | 2.9 | 1,401 |
| 3 | Comparison of Automatic Three-Dimensional Model Builders Using 639 X-ray Structures. Journal of Chemical Information and Computer Sciences, 1994, 34, 1000-1008. | 2.8 | 596 |
| 4 | A new model for calculating atomic charges in molecules. Tetrahedron Letters, 1978, 19, 3181-3184. | 0.7 | 446 |
| 5 | Electronegativity equalization: application and parametrization. Journal of the American Chemical Society, 1985, 107, 829-835. | 6.6 | 429 |
| 6 | Neural Networks in Chemistry. Angewandte Chemie International Edition in English, 1993, 32, 503-527. | 4.4 | 418 |
| 7 | From atoms and bonds to three-dimensional atomic coordinates: automatic model builders. Chemical Reviews, 1993, 93, 2567-2581. | 23.0 | 400 |
| 8 | Autocorrelation of Molecular Surface Properties for Modeling Corticosteroid Binding Globulin and Cytosolic Ah Receptor Activity by Neural Networks. Journal of the American Chemical Society, 1995, 117, 7769-7775. | 6.6 | 325 |
| 9 | The Coding of the Three-Dimensional Structure of Molecules by Molecular Transforms and Its Application to Structure-Spectra Correlations and Studies of Biological Activity. Journal of Chemical Information and Computer Sciences, 1996, 36, 334-344. | 2.8 | 314 |
| 10 | Deriving the 3D structure of organic molecules from their infrared spectra. Vibrational Spectroscopy, 1999, 19, 151-164. | 1.2 | 274 |
| 11 | 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 |
| 12 | Prediction of1H NMR Chemical Shifts Using Neural Networks. Analytical Chemistry, 2002, 74, 80-90. | 3.2 | 178 |
| 13 | Chemical Information in 3D Space. Journal of Chemical Information and Computer Sciences, 1996, 36, 1030-1037. | 2.8 | 176 |
| 14 | A Graph-Based Genetic Algorithm and Its Application to the Multiobjective Evolution of Median Molecules. Journal of Chemical Information and Computer Sciences, 2004, 44, 1079-1087. | 2.8 | 151 |
| 15 | Structure and reaction based evaluation of synthetic accessibility. Journal of Computer-Aided Molecular Design, 2007, 21, 311-325. | 1.3 | 140 |
| 16 | Locating Biologically Active Compounds in Medium-Sized Heterogeneous Datasets by Topological Autocorrelation Vectors:â€‰ Dopamine and Benzodiazepine Agonists. Journal of Chemical Information and Computer Sciences, 1996, 36, 1205-1213. | 2.8 | 138 |
| 17 | Prediction of Aqueous Solubility of Organic Compounds Based on a 3D Structure Representation. Journal of Chemical Information and Computer Sciences, 2003, 43, 429-434. | 2.8 | 138 |
| 18 | Prediction of proton magnetic resonance shifts: The dependence on hydrogen charges obtained by iterative partial equalization of orbital electronegativity. Magnetic Resonance in Chemistry, 1981, 15, 353-360. | 0.7 | 123 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Representation of Molecular Electrostatic Potentials by Topological Feature Maps. Journal of the American Chemical Society, 1994, 116, 4608-4620. | 6.6 | 118 |
| 20 | Computer-Assisted Planning of Organic Syntheses: The Second Generation of Programs. Angewandte Chemie International Edition in English, 1996, 34, 2613-2633. | 4.4 | 104 |
| 21 | Classification of multicomponent analytical data of olive oils using different neural networks. Analytica Chimica Acta, 1994, 292, 219-234. | 2.6 | 102 |
| 22 | New Applications of Computers in Chemistry. Angewandte Chemie International Edition in English, 1979, 18, 111-123. | 4.4 | 98 |
| 23 | Calculation of the Charge Distribution in Conjugated Systems by a Quantification of the Resonance Concept. Angewandte Chemie International Edition in English, 1985, 24, 687-689. | 4.4 | 96 |
| 24 | Ligand-Based Models for the Isoform Specificity of Cytochrome P450 3A4, 2D6, and 2C9 Substrates. Journal of Chemical Information and Modeling, 2007, 47, 1688-1701. | 2.5 | 93 |
| 25 | Superposition of Three-Dimensional Chemical Structures Allowing for Conformational Flexibility by a Hybrid Method. Journal of Chemical Information and Computer Sciences, 1998, 38, 220-232. | 2.8 | 90 |
| 26 | Hash codes for the identification and classification of molecular structure elements. Journal of Computational Chemistry, 1994, 15, 793-813. | 1.5 | 88 |
| 27 | Residual electronegativity - an empirical quantification of polar influences and its application to the proton affinity of amines. Tetrahedron Letters, 1983, 24, 2541-2544. | 0.7 | 83 |
| 28 | A combined application of two different neural network types for the prediction of chemical reactivity. Journal of the American Chemical Society, 1993, 115, 9148-9159. | 6.6 | 82 |
| 29 | Use of the Kohonen Neural Network for Rapid Screening of Ex Vivo Anti-HIV Activity of Styrylquinolines. Journal of Medicinal Chemistry, 2002, 45, 4647-4654. | 2.9 | 82 |
| 30 | Infrared Spectra Simulation of Substituted Benzene Derivatives on the Basis of a 3D Structure Representation. Analytical Chemistry, 1997, 69, 2398-2405. | 3.2 | 80 |
| 31 | The comparison of geometric and electronic properties of molecular surfaces by neural networks: Application to the analysis of corticosteroid-binding globulin activity of steroids. Journal of Computer-Aided Molecular Design, 1996, 10, 521-534. | 1.3 | 79 |
| 32 | Quantitative models of gas-phase proton-transfer reactions involving alcohols, ethers, and their thio analogs. Correlation analyses based on residual electronegativity and effective polarizability. Journal of the American Chemical Society, 1984, 106, 6489-6495. | 6.6 | 75 |
| 33 | Knowledge Discovery in Reaction Databases:Â Landscaping Organic Reactions by a Self-Organizing Neural Network. Journal of the American Chemical Society, 1997, 119, 4033-4042. | 6.6 | 72 |
| 34 | Neural networks and genetic algorithms in drug design. Drug Discovery Today, 2001, 6, 102-108. | 3.2 | 71 |
| 35 | The generation of 3D models of host-guest complexes. Analytica Chimica Acta, 1992, 265, 233-241. | 2.6 | 69 |
| 36 | Prediction of pKa Values for Aliphatic Carboxylic Acids and Alcohols with Empirical Atomic Charge Descriptors. Journal of Chemical Information and Modeling, 2006, 46, 2256-2266. | 2.5 | 66 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Chemoinformatics: a new field with a long tradition. Analytical and Bioanalytical Chemistry, 2006, 384, 57-64. | 1.9 | 65 |
| 38 | Chemoinformatics: Achievements and Challenges, a Personal View. Molecules, 2016, 21, 151. | 1.7 | 63 |
| 39 | Neuronale Netze in der Chemie. Angewandte Chemie, 1993, 105, 510-536. | 1.6 | 60 |
| 40 | Neural networks as data mining tools in drug design. Journal of Physical Organic Chemistry, 2003, 16, 232-245. | 0.9 | 60 |
| 41 | The Principle of Minimum Chemical Distance(PMCD). Angewandte Chemie International Edition in English, 1980, 19, 495-505. | 4.4 | 59 |
| 42 | New Description of Molecular Chirality and Its Application to the Prediction of the Preferred Enantiomer in Stereoselective Reactions. Journal of Chemical Information and Computer Sciences, 2001, 41, 369-375. | 2.8 | 58 |
| 43 | Sesquiterpene lactone-based classification of three Asteraceae tribes: a study based on self-organizing neural networks applied to chemosystematics. Phytochemistry, 2005, 66, 345-353. | 1.4 | 58 |
| 44 | Prediction of Aqueous Solubility of Organic Compounds by Topological Descriptors. QSAR and Combinatorial Science, 2003, 22, 821-829. | 1.5 | 57 |
| 45 | Self-Organizing Maps for Identification of New Inhibitors of P-Glycoprotein. Journal of Medicinal Chemistry, 2007, 50, 1698-1702. | 2.9 | 55 |
| 46 | Development of a Structural Model for NF-Î°B Inhibition of Sesquiterpene Lactones Using Self-Organizing Neural Networks. Journal of Medicinal Chemistry, 2006, 49, 2241-2252. | 2.9 | 54 |
| 47 | An Algorithm for the Perception of Synthetically Important Rings. Journal of Chemical Information and Computer Sciences, 1979, 19, 43-48. | 2.8 | 52 |
| 48 | Classification of Organic Reactions:â€‰ Similarity of Reactions Based on Changes in the Electronic Features of Oxygen Atoms at the Reaction Sites1. Journal of Chemical Information and Computer Sciences, 1998, 38, 210-219. | 2.8 | 52 |
| 49 | Of Molecules and Humans. Journal of Medicinal Chemistry, 2006, 49, 6429-6434. | 2.9 | 52 |
| 50 | Simulation of Organic Reactions:â€‰ From the Degradation of Chemicals to Combinatorial Synthesis. Journal of Chemical Information and Computer Sciences, 2000, 40, 482-494. | 2.8 | 51 |
| 51 | Impact of Conformational Flexibility on Three-Dimensional Similarity Searching Using Correlation Vectors. Journal of Chemical Information and Modeling, 2006, 46, 2324-2332. | 2.5 | 51 |
| 52 | 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 |
| 53 | Chlor-, Brom- und Jod-cyclooctatetraen: Darstellung und einige Reaktionen. Chemische Berichte, 1971, 104, 2412-2419. | 0.2 | 49 |
| 54 | Enabling the exploration of biochemical pathways. Organic and Biomolecular Chemistry, 2004, 2, 3226-3237. | 1.5 | 49 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Prediction of enantiomeric selectivity in chromatography. Journal of Molecular Graphics and Modelling, 2002, 20, 373-388. | 1.3 | 48 |
| 56 | Automated derivation of reaction rules for the EROS 6.0 system for reaction prediction. Analytica Chimica Acta, 1990, 235, 163-168. | 2.6 | 46 |
| 57 | Chemistry in Times of Artificial Intelligence. ChemPhysChem, 2020, 21, 2233-2242. | 1.0 | 46 |
| 58 | Similarity concepts for the planning of organic reactions and syntheses. Journal of Chemical Information and Computer Sciences, 1992, 32, 700-712. | 2.8 | 44 |
| 59 | Prediction of three-dimensional molecular structures using information from infrared spectra. Analytica Chimica Acta, 2000, 420, 145-154. | 2.6 | 44 |
| 60 | Prediction of Enantiomeric Excess in a Combinatorial Library of Catalytic Enantioselective Reactions. ACS Combinatorial Science, 2005, 7, 298-301. | 3.3 | 43 |
| 61 | Overcoming the Limitations of a Connection Table Description:â€‰ A Universal Representation of Chemical Species. Journal of Chemical Information and Computer Sciences, 1997, 37, 705-714. | 2.8 | 42 |
| 62 | Use of Structure Descriptors To Discriminate between Modes of Toxic Action of Phenols. Journal of Chemical Information and Modeling, 2005, 45, 200-208. | 2.5 | 42 |
| 63 | Uncovering metabolic pathways relevant to phenotypic traits of microbial genomes. Genome Biology, 2009, 10, R28. | 13.9 | 39 |
| 64 | Chirality Codes and Molecular Structure. Journal of Chemical Information and Computer Sciences, 2004, 44, 831-836. | 2.8 | 37 |
| 65 | New empirical models of substituent polarisability and their application to stabilisation effects in positively charged species. Tetrahedron Letters, 1983, 24, 2537-2540. | 0.7 | 34 |
| 66 | Comparison of Different Classification Methods Applied to a Mode of Toxic Action Data Set. QSAR and Combinatorial Science, 2004, 23, 779-791. | 1.5 | 33 |
| 67 | Combining Chemoinformatics with Bioinformatics: In Silico Prediction of Bacterial Flavor-Forming Pathways by a Chemical Systems Biology Approach â€œReverse Pathway Engineeringâ€• PLoS ONE, 2014, 9, e84769. | 1.1 | 33 |
| 68 | Comparison of structurally different allosteric modulators of muscarinic receptors by self-organizing neural networks. Journal of Molecular Graphics, 1996, 14, 185-193. | 1.7 | 32 |
| 69 | The Search for the Spatial and Electronic Requirements of a Drug. Journal of Molecular Modeling, 2000, 6, 358-378. | 0.8 | 26 |
| 70 | ChemInform - an integrated information system on chemical reactions. Journal of Chemical Information and Computer Sciences, 1990, 30, 400-402. | 2.8 | 25 |
| 71 | Computer-assisted synthesis and reaction planning in combinatorial chemistry. Journal of Computer - Aided Molecular Design, 2000, 20, 245-264. | 1.0 | 25 |
| 72 | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Classification of Mixtures of Chinese Herbal Medicines Based on a Selfâ€organizing Map (SOM). Molecular Informatics, 2016, 35, 109-115. | 1.4 | 22 |
| 74 | Computer-assisted prediction of the degradation of chemicals: hydrolysis of amides and benzoylphenylureas. Journal of the Chemical Society Perkin Transactions II, 1995, , 193-204. | 0.9 | 21 |
| 75 | Correlation analyses of the aqueous-phase acidities of alcohols and gem-diols, and of carbonyl hydration equilibria using electronic and structural parameters. Journal of the Chemical Society Perkin Transactions II, 1986, , 455. | 0.9 | 19 |
| 76 | 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 |
| 77 | Physicochemical Effects in the Representation of Molecular Structures for Drug Designing. Mini-Reviews in Medicinal Chemistry, 2003, 3, 789-796. | 1.1 | 17 |
| 78 | 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 |
| 79 | Computing target complexity. Nature Chemistry, 2015, 7, 619-620. | 6.6 | 17 |
| 80 | Fingal: A Novel Approach to Geometric Fingerprinting and a Comparative Study of Its Application to 3D-QSAR Modelling. QSAR and Combinatorial Science, 2005, 24, 480-484. | 1.5 | 13 |
| 81 | ComputergestÃ¼tzte Planung organischâ€chemischer Synthesen: die zweite Programmgeneration. Angewandte Chemie, 1995, 107, 2807-2829. | 1.6 | 12 |
| 82 | Modeling chemical reactions for drug design. Journal of Computer-Aided Molecular Design, 2007, 21, 33-52. | 1.3 | 11 |
| 83 | A quantitative description of fundamental polar reaction types. Proton- and hydride-transfer reactions connecting alcohols and carbonyl compounds in the gas phase. Journal of the Chemical Society Perkin Transactions II, 1986, , 447. | 0.9 | 10 |
| 84 | Query Generation to Search for Inhibitors of Enzymatic Reactions. Journal of Chemical Information and Modeling, 2006, 46, 2333-2341. | 2.5 | 9 |
| 85 | Solved and Unsolved Problems of Chemoinformatics. Molecular Informatics, 2014, 33, 454-457. | 1.4 | 8 |
| 86 | 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 |
| 87 | Steroid binding by antibodies and artificial receptors: exploration of theoretical methods to determine the origins of binding affinities and specificities. Journal of Computer-Aided Molecular Design, 2000, 14, 611-629. | 1.3 | 4 |
| 88 | Chemistry on the Internet. , 0, , 794-843. | | 4 |
| 89 | Explorations into Chemical Reactions and Biochemical Pathways. Molecular Informatics, 2016, 35, 588-592. | 1.4 | 1 |
| 90 | Leaving us with fond memories, smiles, SMILES and, alas, tears: a tribute to David Weininger, 1952â€“2016. Journal of Computer-Aided Molecular Design, 2018, 32, 313-319. | 1.3 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | Descriptors for Chemical Compounds. , 0, , 977-979. | | 1 |
| 92 | Chemical Reactions. , 2018, , 83-83. | | 0 |
| 93 | [Special Issue for Honor Award dedicating to Prof Kimito Funatsu]Kimito Funatsu â€“ The Driving Force of Chemoinformatics in Japan. Journal of Computer Aided Chemistry, 2019, 20, 32-34. | 0.3 | 0 |
| 94 | Methods for Data Analysis. , 0, , 1079-1081. | | 0 |
| 95 | The Data. , 0, , 389-391. | | 0 |
| 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 |