# Kimito Funatsu

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/6877828/publications.pdf

Version: 2024-02-01

| 203 | 5,922 | 126708 | 88477 |
|---|---|---|---|
| papers | citations | 33 h-index | 70 g-index |

| 209 | 209 | 209 | 6090 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | MassBank: a public repository for sharing mass spectral data for life sciences. Journal of Mass Spectrometry, 2010, 45, 703-714. | 0.7 | 1,831 |
| 2 | Rethinking drug design in the artificial intelligence era. Nature Reviews Drug Discovery, 2020, 19, 353-364. | 21.5 | 394 |
| 3 | GA Strategy for Variable Selection in QSAR Studies:â€‰GA-Based PLS Analysis of Calcium Channel Antagonists. Journal of Chemical Information and Computer Sciences, 1997, 37, 306-310. | 2.8 | 218 |
| 4 | Development of a new soft sensor method using independent component analysis and partial least squares. AICHE Journal, 2009, 55, 87-98. | 1.8 | 134 |
| 5 | Genetic algorithmâ€based wavelength selection method for spectral calibration. Journal of Chemometrics, 2011, 25, 10-19. | 0.7 | 123 |
| 6 | Adaptive soft sensor based on online support vector regression and Bayesian ensemble learning for various states in chemical plants. Chemometrics and Intelligent Laboratory Systems, 2014, 137, 57-66. | 1.8 | 94 |
| 7 | Maintenance-free soft sensor models with time difference of process variables. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 312-317. | 1.8 | 85 |
| 8 | Inverse QSPR/QSAR Analysis for Chemical Structure Generation (from y to x). Journal of Chemical Information and Modeling, 2016, 56, 286-299. | 2.5 | 83 |
| 9 | SOPHIA, a Knowledge Base-Guided Reaction Prediction System - Utilization of a Knowledge Base Derived from a Reaction Database. Journal of Chemical Information and Computer Sciences, 1995, 35, 34-44. | 2.8 | 81 |
| 10 | GA Strategy for Variable Selection in QSAR Studies:â€‰Application of GA-Based Region Selection to a 3D-QSAR Study of Acetylcholinesterase Inhibitors. Journal of Chemical Information and Computer Sciences, 1999, 39, 112-120. | 2.8 | 77 |
| 11 | Application of online support vector regression for soft sensors. AICHE Journal, 2014, 60, 600-612. | 1.8 | 74 |
| 12 | Further development of structure generation in the automated structure elucidation system CHEMICS. Journal of Chemical Information and Modeling, 1988, 28, 18-28. | 2.5 | 71 |
| 13 | Recent Advances in the Automated Structure Elucidation System, CHEMICS. Utilization of Two-Dimensional NMR Spectral Information and Development of Peripheral Functions for Examination of Candidates. Journal of Chemical Information and Computer Sciences, 1996, 36, 190-204. | 2.8 | 71 |
| 14 | Classification of the Degradation of Soft Sensor Models and Discussion on Adaptive Models. AICHE Journal, 2013, 59, 2339-2347. | 1.8 | 66 |
| 15 | Applicability domains and accuracy of prediction of soft sensor models. AICHE Journal, 2011, 57, 1506-1513. | 1.8 | 64 |
| 16 | A soft sensor method based on values predicted from multiple intervals of time difference for improvement and estimation of prediction accuracy. Chemometrics and Intelligent Laboratory Systems, 2011, 109, 197-206. | 1.8 | 61 |
| 17 | A Novel Approach to Retrosynthetic Analysis Using Knowledge Bases Derived from Reaction Databases. Journal of Chemical Information and Computer Sciences, 1999, 39, 316-325. | 2.8 | 57 |
| 18 | Development of Soft Sensor Models Based on Time Difference of Process Variables with Accounting for Nonlinear Relationship. Industrial & Engineering Chemistry Research, 2011, 50, 10643-10651. | 1.8 | 55 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Fast optimization of hyperparameters for support vector regression models with highly predictive ability. Chemometrics and Intelligent Laboratory Systems, 2015, 142, 64-69. | 1.8 | 55 |
| 20 | 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 |
| 21 | GA Strategy for Variable Selection in QSAR Studies:â€‰ GA-Based Region Selection for CoMFA Modeling. Journal of Chemical Information and Computer Sciences, 1998, 38, 276-282. | 2.8 | 50 |
| 22 | Novel soft sensor method for detecting completion of transition in industrial polymer processes. Computers and Chemical Engineering, 2011, 35, 1135-1142. | 2.0 | 50 |
| 23 | Development of a New Regression Analysis Method Using Independent Component Analysis. Journal of Chemical Information and Modeling, 2008, 48, 534-541. | 2.5 | 49 |
| 24 | Applicability Domain Based on Ensemble Learning in Classification and Regression Analyses. Journal of Chemical Information and Modeling, 2014, 54, 2469-2482. | 2.5 | 48 |
| 25 | Ensemble locally weighted partial least squares as a justâ€inâ€time modeling method. AICHE Journal, 2016, 62, 717-725. | 1.8 | 44 |
| 26 | Computer-assisted organic synthesis design and reaction prediction system, â€œAIPHOSâ€. Tetrahedron Computer Methodology, 1988, 1, 27-37. | 0.2 | 41 |
| 27 | Exhaustive Structure Generation for Inverseâ€QSPR/QSAR. Molecular Informatics, 2010, 29, 111-125. | 1.4 | 40 |
| 28 | A new process variable and dynamics selection method based on a genetic algorithmâ€based wavelength selection method. AICHE Journal, 2012, 58, 1829-1840. | 1.8 | 40 |
| 29 | Adaptive soft sensor model using online support vector regression with time variable and discussion of appropriate hyperparameter settings and window size. Computers and Chemical Engineering, 2013, 58, 288-297. | 2.0 | 40 |
| 30 | The Recent Trend in QSAR Modeling - Variable Selection and 3D-QSAR Methods. Current Computer-Aided Drug Design, 2007, 3, 254-262. | 0.8 | 38 |
| 31 | Plasma and Hepatic Concentrations of Chemicals after Virtual Oral Administrations Extrapolated Using Rat Plasma Data and Simple Physiologically Based Pharmacokinetic Models. Chemical Research in Toxicology, 2019, 32, 211-218. | 1.7 | 38 |
| 32 | Comparison and improvement of the predictability and interpretability with ensemble learning models in QSPR applications. Journal of Cheminformatics, 2020, 12, 19. | 2.8 | 38 |
| 33 | Database monitoring index for adaptive soft sensors and the application to industrial process. AICHE Journal, 2014, 60, 160-169. | 1.8 | 37 |
| 34 | Determination and prediction of permeability across intestinal epithelial cell monolayer of a diverse range of industrial chemicals/drugs for estimation of oral absorption as a putative marker of hepatotoxicity. Toxicology Reports, 2020, 7, 149-154. | 1.6 | 36 |
| 35 | Varying resonance demands in substituent effects. Acetolysis of neophyl p-bromobenzenesulfonates. Tetrahedron, 1987, 43, 307-316. | 1.0 | 34 |
| 36 | Introduction of two-dimensional NMR spectral information to an automated structure elucidation system, CHEMICS. Utilization of 2D-INADEQUATE information. Journal of Chemical Information and Computer Sciences, 1989, 29, 6-11. | 2.8 | 33 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | New molecular surface-based 3D-QSAR method using Kohonen neural network and 3-way PLS. Computers & Chemistry, 2002, 26, 583-589. | 1.2 | 33 |
| 38 | Moving Window and Just-in-Time Soft Sensor Model Based on Time Differences Considering a Small Number of Measurements. Industrial & Engineering Chemistry Research, 2015, 54, 700-704. | 1.8 | 33 |
| 39 | Computer-assisted structure/taste studies on sulfamates by pattern recognition methods. Analytica Chimica Acta, 1986, 184, 143-149. | 2.6 | 32 |
| 40 | Further Development of a Reaction Generator in the SOPHIA System for Organic Reaction Prediction. Knowledge-Guided Addition of Suitable Atoms and/or Atomic Groups to Product Skeleton. Journal of Chemical Information and Computer Sciences, 1996, 36, 173-184. | 2.8 | 32 |
| 41 | Non-Linear Modeling and Chemical Interpretation with Aid of Support Vector Machine and Regression. Current Computer-Aided Drug Design, 2010, 6, 24-36. | 0.8 | 32 |
| 42 | Quantitative Structureâ^'Activity Relationships of the Synthetic Substrates for Elastase Enzyme Using Nonlinear Partial Least Squares Regression. Journal of Chemical Information and Computer Sciences, 1996, 36, 185-189. | 2.8 | 31 |
| 43 | Solvent Effects on the Solvolysis of Neophyl Tosylates. Bulletin of the Chemical Society of Japan, 1992, 65, 46-54. | 2.0 | 28 |
| 44 | Systematic Generation of Chemical Structures for Rational Drug Design Based on QSAR Models. Current Computer-Aided Drug Design, 2011, 7, 1-9. | 0.8 | 28 |
| 45 | Physiologically Based Pharmacokinetic Models Predicting Renal and Hepatic Concentrations of Industrial Chemicals after Virtual Oral Doses in Rats. Chemical Research in Toxicology, 2020, 33, 1736-1751. | 1.7 | 27 |
| 46 | Novel Canonical Coding Method for Representation of Three-Dimensional Structures. Journal of Chemical Information and Computer Sciences, 2000, 40, 622-630. | 2.8 | 26 |
| 47 | Nonlinear Partial Least Squares Modeling of Phenyl Alkylamines with the Monoamine Oxidase Inhibitory Activities. Journal of Chemical Information and Computer Sciences, 1996, 36, 1025-1029. | 2.8 | 24 |
| 48 | Nonlinear regression method with variable region selection and application to soft sensors. Chemometrics and Intelligent Laboratory Systems, 2013, 121, 26-32. | 1.8 | 24 |
| 49 | Multivariate Statistical Process Control Method Including Soft Sensors for Both Early and Accurate Fault Detection. Industrial & Engineering Chemistry Research, 2014, 53, 8553-8564. | 1.8 | 24 |
| 50 | Ringâ€Systemâ€Based Exhaustive Structure Generation for Inverseâ€QSPR/QSAR. Molecular Informatics, 2014, 33, 764-778. | 1.4 | 24 |
| 51 | Substituent Effects. XVI. Acetolysis of 2-Phenylethyl Tosylates. Bulletin of the Chemical Society of Japan, 1987, 60, 1091-1095. | 2.0 | 23 |
| 52 | Chemography of Natural Product Space. Planta Medica, 2015, 81, 429-435. | 0.7 | 23 |
| 53 | In Silico Prediction of Input Parameters for Simplified Physiologically Based Pharmacokinetic Models for Estimating Plasma, Liver, and Kidney Exposures in Rats after Oral Doses of 246 Disparate Chemicals. Chemical Research in Toxicology, 2021, 34, 507-513. | 1.7 | 23 |
| 54 | Application of infrared data analysis based on symbolic logic in automated structure elucidation by chemics. Analytica Chimica Acta, 1989, 220, 155-169. | 2.6 | 22 |

| # | Article | IF | Citations |
|---|---|---|---|
| 55 | Representation of Molecular Configurations by CAST Coding Method. Journal of Chemical Information and Computer Sciences, 2001, 41, 1106-1112. | 2.8 | 20 |
| 56 | Chemical-Space-Based de Novo Design Method To Generate Drug-Like Molecules. Journal of Chemical Information and Modeling, 2016, 56, 1885-1893. | 2.5 | 20 |
| 57 | Optimization of the Inner Relation Function of QPLS Using Genetic Algorithm. Journal of Chemical Information and Computer Sciences, 1997, 37, 1115-1121. | 2.8 | 19 |
| 58 | Applicability domain of soft sensor models based on oneâ€€class support vector machine. AICHE Journal, 2013, 59, 2046-2050. | 1.8 | 19 |
| 59 | Automatic recognition of reaction site in organic chemical reactions. Tetrahedron Computer Methodology, 1988, 1, 53-69. | 0.2 | 17 |
| 60 | Introduction of NOE data to an automated structure elucidation system, CHEMICS. Three-dimensional structure elucidation using the distance geometry method. Journal of Chemical Information and Computer Sciences, 1994, 34, 745-751. | 2.8 | 17 |
| 61 | Application of the Novel Molecular Alignment Method Using the Hopfield Neural Network to 3D-QSAR. Journal of Chemical Information and Computer Sciences, 2003, 43, 1396-1402. | 2.8 | 17 |
| 62 | Quantitative Prediction of Regioselectivity Toward Cytochrome P450/3A4 Using Machine Learning Approaches. Molecular Informatics, 2010, 29, 243-249. | 1.4 | 17 |
| 63 | Criterion for Evaluating the Predictive Ability of Nonlinear Regression Models without Cross-Validation. Journal of Chemical Information and Modeling, 2013, 53, 2341-2348. | 2.5 | 17 |
| 64 | Multi-way PLS modeling of structureâ€“activity data by incorporating electrostatic and lipophilic potentials on molecular surface. Computational Biology and Chemistry, 2003, 27, 381-386. | 1.1 | 16 |
| 65 | Development of a New De Novo Design Algorithm for Exploring Chemical Space. Molecular Informatics, 2014, 33, 779-789. | 1.4 | 16 |
| 66 | Random Forest Approach to QSPR Study of Fluorescence Properties Combining Quantum Chemical Descriptors and Solvent Conditions. Journal of Fluorescence, 2018, 28, 695-706. | 1.3 | 16 |
| 67 | Substituent effect on the acetolysis of 2-phenylethyl tosylate. Tetrahedron Letters, 1983, 24, 2177-2180. | 0.7 | 15 |
| 68 | A Novel Method for Characterization of Three-Dimensional Reaction Fields Based on Electrostatic and Steric Interactions toward the Goal of Quantitative Analysis and Understanding of Organic Reactions. Journal of Chemical Information and Computer Sciences, 1999, 39, 671-678. | 2.8 | 15 |
| 69 | Discrimination of Poly(vinyl chloride) Samples with Different Plasticizers and Prediction of Plasticizer Contents in Poly(vinyl chloride) Using Near-infrared Spectroscopy and Neural-network Analysis.. Analytical Sciences, 2003, 19, 309-312. | 0.8 | 15 |
| 70 | Chemoinformatics â€“ An Important Scientific Discipline. Journal of Computer Chemistry Japan, 2006, 5, 53-58. | 0.0 | 15 |
| 71 | 2D and 3D QSAR studies of the receptor binding affinity of progestins. Journal of the Brazilian Chemical Society, 2010, 21, 872-881. | 0.6 | 15 |
| 72 | Estimation of predictive accuracy of soft sensor models based on data density. Chemometrics and Intelligent Laboratory Systems, 2013, 128, 111-117. | 1.8 | 15 |

| # | Article | IF | Citations |
|---|---|---|---|
| 73 | Discussion on Time Difference Models and Intervals of Time Difference for Application of Soft Sensors. Industrial & Engineering Chemistry Research, 2013, 52, 1322-1334. | 1.8 | 15 |
| 74 | Selective Use of Adaptive Soft Sensors Based on Process State. Industrial & Engineering Chemistry Research, 2014, 53, 15962-15968. | 1.8 | 15 |
| 75 | Smoothing-Combined Soft Sensors for Noise Reduction and Improvement of Predictive Ability. Industrial & Engineering Chemistry Research, 2015, 54, 12630-12638. | 1.8 | 15 |
| 76 | Combined generative topographic mapping and graph theory unsupervised approach for nonlinear fault identification. AICHE Journal, 2015, 61, 1559-1571. | 1.8 | 15 |
| 77 | Visualization of Molecular Selectivity and Structure Generation for Selective Dopamine Inhibitors. Molecular Informatics, 2010, 29, 793-800. | 1.4 | 14 |
| 78 | Physical and statistical model for predicting a transmembrane pressure jump for a membrane bioreactor. Chemometrics and Intelligent Laboratory Systems, 2013, 121, 66-74. | 1.8 | 14 |
| 79 | Improvement of iterative optimization technology (for process analytical technology) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 5 spectra. Chemometrics and Intelligent Laboratory Systems, 2015, 147, 176-184. | 1.8 | 14 |
| 80 | Ring system-based chemical graph generation for de novo molecular design. Journal of Computer-Aided Molecular Design, 2016, 30, 425-446. | 1.3 | 14 |
| 81 | Soft Sensor Modeling for Identifying Significant Process Variables with Time Delays. Industrial & Engineering Chemistry Research, 2020, 59, 12156-12163. | 1.8 | 14 |
| 82 | Prediction of permeability across intestinal cell monolayers for 219 disparate chemicals using in vitro experimental coefficients in a pH gradient system and in silico analyses by trivariate linear regressions and machine learning. Biochemical Pharmacology, 2021, 192, 114749. | 2.0 | 14 |
| 83 | Novel Alignment Method of Small Molecules Using the Hopfield Neural Network. Journal of Chemical Information and Computer Sciences, 2003, 43, 1390-1395. | 2.8 | 13 |
| 84 | Tailored scoring function of Trypsinâ€“benzamidine complex using COMBINE descriptors and support vector regression. Chemometrics and Intelligent Laboratory Systems, 2008, 92, 145-151. | 1.8 | 13 |
| 85 | Adaptive database management based on the database monitoring index for long-term use of adaptive soft sensors. Chemometrics and Intelligent Laboratory Systems, 2015, 146, 179-185. | 1.8 | 13 |
| 86 | Simultaneous determination of bioactive conformations and alignment rules by multi-way PLS modeling. Computational Biology and Chemistry, 2003, 27, 211-216. | 1.1 | 12 |
| 87 | Evolution of PLS for Modeling SAR and omics Data. Molecular Informatics, 2012, 31, 766-775. | 1.4 | 12 |
| 88 | Visualization of Models Predicting Transmembrane Pressure Jump for Membrane Bioreactor. Industrial & Engineering Chemistry Research, 2012, 51, 9679-9686. | 1.8 | 12 |
| 89 | Flour concentration prediction using GAPLS and GAWLS focused on data sampling issues and applicability domain. Chemometrics and Intelligent Laboratory Systems, 2014, 137, 33-46. | 1.8 | 12 |
| 90 | De novo Drug Design â€“ Ye olde Scoring Problem Revisited. Molecular Informatics, 2017, 36, 1681031. | 1.4 | 12 |

| # | Article | IF | Citations |
|---|---|---|---|
| 91 | On Generative Topographic Mapping and Graph Theory combined approach for unsupervised non-linear data visualization and fault identification. Computers and Chemical Engineering, 2017, 98, 113-127. | 2.0 | 12 |
| 92 | A chemometric approach to prediction of transmembrane pressure in membrane bioreactors. Chemometrics and Intelligent Laboratory Systems, 2013, 126, 30-37. | 1.8 | 11 |
| 93 | Random Forest Model with Combined Features: A Practical Approach to Predict Liquidâ€crystalline Property. Molecular Informatics, 2019, 38, e1800095. | 1.4 | 11 |
| 94 | Comparing predictive ability of QSAR/QSPR models using 2D and 3D molecular representations. Journal of Computer-Aided Molecular Design, 2021, 35, 179-193. | 1.3 | 11 |
| 95 | Prediction of Polyethylene Density by Near-Infrared Spectroscopy Combined with Neural Network Analysis. Journal of Computer Chemistry Japan, 2003, 2, 33-40. | 0.0 | 11 |
| 96 | Advanced PLS Techniques in Chemoinformatics Studies. Current Computer-Aided Drug Design, 2010, 6, 103-127. | 0.8 | 10 |
| 97 | Detection of nonlinearity in soil property prediction models based on near-infrared spectroscopy. Chemometrics and Intelligent Laboratory Systems, 2017, 167, 139-151. | 1.8 | 10 |
| 98 | Nonlinear CoMFA using QPLS as a Novel 3D-QSAR Approach. QSAR and Combinatorial Science, 1997, 16, 219-223. | 1.4 | 9 |
| 99 | Application of data mining to quantitative structure-activity relationship using rough set theory. Chemometrics and Intelligent Laboratory Systems, 2009, 99, 66-70. | 1.8 | 9 |
| 100 | New description of proteinâ€“ligand interactions using a spherical self-organizing map. Bioorganic and Medicinal Chemistry, 2012, 20, 5410-5415. | 1.4 | 9 |
| 101 | Development of high predictive soft sensor method and the application to industrial polymer processes. Asia-Pacific Journal of Chemical Engineering, 2012, 7, S39. | 0.8 | 9 |
| 102 | Data density-based fault detection and diagnosis with nonlinearities between variables and multimodal data distributions. Chemometrics and Intelligent Laboratory Systems, 2015, 147, 58-65. | 1.8 | 9 |
| 103 | Preparation of comprehensive data from huge data sets for predictive soft sensors. Chemometrics and Intelligent Laboratory Systems, 2016, 153, 75-81. | 1.8 | 9 |
| 104 | Finding Chemical Structures Corresponding to a Set of Coordinates in Chemical Descriptor Space. Molecular Informatics, 2017, 36, 1700030. | 1.4 | 9 |
| 105 | Three-Dimensional Activity Landscape Models of Different Design and Their Application to Compound Mapping and Potency Prediction. Journal of Chemical Information and Modeling, 2019, 59, 993-1004. | 2.5 | 9 |
| 106 | Exploring Topological Pharmacophore Graphs for Scaffold Hopping. Journal of Chemical Information and Modeling, 2020, 60, 2073-2081. | 2.5 | 9 |
| 107 | An Updated In Silico Prediction Method for Volumes of Systemic Circulation of 323 Disparate Chemicals for Use in Physiologically Based Pharmacokinetic Models to Estimate Plasma and Tissue Concentrations after Oral Doses in Rats. Chemical Research in Toxicology, 2021, 34, 2180-2183. | 1.7 | 9 |
| 108 | Prediction of Reaction Yield for Buchwaldâ€Hartwig Crossâ€coupling Reactions Using Deep Learning. Molecular Informatics, 2022, 41, e2100156. | 1.4 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 109 | Novel Computational Approaches in QSAR and Molecular Design Based on GA, Multi-Way PLS and NN. Current Computer-Aided Drug Design, 2005, 1, 129-145. | 0.8 | 9 |
| 110 | Development of Drug-likeness Model and Its Visualization. Journal of Computer Aided Chemistry, 2008, 9, 70-80. | 0.3 | 8 |
| 111 | Application of the mol2vec Technology to Largeâ€size Data Visualization and Analysis. Molecular Informatics, 2020, 39, e1900170. | 1.4 | 8 |
| 112 | Bayesian Classification of Cytochrome P450 3A4 Substrates/Non-substrates and Color Mapping for Chemical Interpretation. Journal of Computer Aided Chemistry, 2010, 11, 19-24. | 0.3 | 8 |
| 113 | Adaptive Soft Sensor Model Using Online Support Vector Regression with Time Variable and Discussion of Appropriate Parameter Settings. Procedia Computer Science, 2013, 22, 580-589. | 1.2 | 7 |
| 114 | Strategic parameter search method based on prediction errors and data density for efficient product design. Chemometrics and Intelligent Laboratory Systems, 2013, 127, 70-79. | 1.8 | 7 |
| 115 | Strategy of Structure Generation within Applicability Domains with One-Class Support Vector Machine. Bulletin of the Chemical Society of Japan, 2015, 88, 981-988. | 2.0 | 7 |
| 116 | Classification of drug tablets using hyperspectral imaging and wavelength selection with a GAWLS method modified for classification. International Journal of Pharmaceutics, 2015, 491, 130-135. | 2.6 | 7 |
| 117 | Partial constrained least squares (PCLS) and application in soft sensor. Chemometrics and Intelligent Laboratory Systems, 2018, 177, 64-73. | 1.8 | 7 |
| 118 | Exploring Alternative Strategies for the Identification of Potent Compounds Using Support Vector Machine and Regression Modeling. Journal of Chemical Information and Modeling, 2019, 59, 983-992. | 2.5 | 7 |
| 119 | Ligandâ€based Activity Cliff Prediction Models with Applicability Domain. Molecular Informatics, 2020, 39, e2000103. | 1.4 | 7 |
| 120 | Exploring differential evolution for inverse QSAR analysis. F1000Research, 2017, 6, 1285. | 0.8 | 7 |
| 121 | Advanced PLS Techniques in Chemometrics and Their Applications to Molecular Design. , 2011, , 145-168. | | 7 |
| 122 | Molecular centrality for synthetic design of convergent reactions. Tetrahedron, 2008, 64, 4602-4612. | 1.0 | 6 |
| 123 | Development of a New Index to Monitor Database for Soft Sensors. Journal of Computer Aided Chemistry, 2013, 14, 11-22. | 0.3 | 6 |
| 124 | Prediction of Proteinï£¿Protein Interaction Pocket Using Lâ€shaped PLS Approach and Its Visualizations by Generative Topographic Mapping. Molecular Informatics, 2014, 33, 65-72. | 1.4 | 6 |
| 125 | Iterative optimization technology combined with wavelength selection based on excess absorption for a process analytical technology calibrationâ€“minimum approach. Chemometrics and Intelligent Laboratory Systems, 2016, 156, 137-147. | 1.8 | 6 |
| 126 | Development of R-Group Fingerprints Based on the Local Landscape from an Attachment Point of a Molecular Structure. Journal of Chemical Information and Modeling, 2019, 59, 2656-2663. | 2.5 | 6 |

| # | Article | IF | Citations |
|---|---|---|---|
| 127 | Sparse Topological Pharmacophore Graphs for Interpretable Scaffold Hopping. Journal of Chemical Information and Modeling, 2021, 61, 3348-3360. | 2.5 | 6 |
| 128 | Interpretation of Ligand-Based Activity Cliff Prediction Models Using the Matched Molecular Pair Kernel. Molecules, 2021, 26, 4916. | 1.7 | 6 |
| 129 | Automatic Determination Method Based on Cross-Validation for Optimal Intervals of Time Difference. Journal of Chemical Engineering of Japan, 2013, 46, 219-225. | 0.3 | 6 |
| 130 | Classification and Prediction of Reagents' Roles by FRAU System with Self-Organizing Neural Network Model. Bulletin of the Chemical Society of Japan, 2000, 73, 1955-1965. | 2.0 | 5 |
| 131 | Application of Rough Set Theory to High Throughput Screening Data for Rational Selection of Lead Compounds. Chem-Bio Informatics Journal, 2008, 8, 85-95. | 0.1 | 5 |
| 132 | A New Method for Mapping the Molecular Surface of a Protein Structure Using a Spherical Selfâ€Organizing Map. Molecular Informatics, 2012, 31, 161-166. | 1.4 | 5 |
| 133 | Applicability Domains and Consistent Structure Generation. Molecular Informatics, 2017, 36, 1600032. | 1.4 | 5 |
| 134 | Practical Models for Predicting the Emission Peak Wavelengths of Inorganic Phosphors Based on Stoichiometric Information. Chemistry Letters, 2017, 46, 1482-1485. | 0.7 | 5 |
| 135 | Structure Modification toward Applicability Domain of a QSAR/QSPR Model Considering Activity/Property. Molecular Informatics, 2017, 36, 1700076. | 1.4 | 5 |
| 136 | Development of a Novel Spectra Analysis Method to Construct Accurate NIR Models. Journal of Computer Aided Chemistry, 2014, 15, 1-9. | 0.3 | 5 |
| 137 | Governing Factors for Carbon Nanotube Dispersion in Organic Solvents Estimated by Machine Learning. Advanced Materials Interfaces, 2022, 9, . | 1.9 | 5 |
| 138 | Development of the computer software. Journal of Computer Aided Chemistry, 2005, 6, 90-96. | 0.3 | 4 |
| 139 | Core Electron Binding Energy (CEBE) as Descriptors in Quantitative Structureâ€“Activity Relationship (QSAR) Analysis of Cytotoxicities of a Series of Simple Phenols. QSAR and Combinatorial Science, 2007, 26, 378-384. | 1.5 | 4 |
| 140 | Automatic Database Monitoring for Process Control Systems. Lecture Notes in Computer Science, 2014, , 410-419. | 1.0 | 4 |
| 141 | A Novel Calibration-Minimum Method for Prediction of Mole Fraction in Non-Ideal Mixture. AAPS PharmSciTech, 2017, 18, 595-604. | 1.5 | 4 |
| 142 | Exploring differential evolution for inverse QSAR analysis. F1000Research, 2017, 6, 1285. | 0.8 | 4 |
| 143 | Identification of Bioactive Scaffolds Based on QSAR Models. Molecular Informatics, 2018, 37, 1700103. | 1.4 | 4 |
| 144 | Evaluation of different virtual screening strategies on the basis of compound sets with characteristic core distributions and dissimilarity relationships. Journal of Computer-Aided Molecular Design, 2019, 33, 729-743. | 1.3 | 4 |

| # | Article | IF | Citations |
|---|---|---|---|
| 145 | Iterative Screening Methods for Identification of Chemical Compounds with Specific Values of Various Properties. Journal of Chemical Information and Modeling, 2019, 59, 2626-2641. | 2.5 | 4 |
| 146 | Ensemble Machine Learning and Applicability Domain Estimation for Fluorescence Properties and its Application to Structural Design. Journal of Computer Aided Chemistry, 2019, 20, 7-17. | 0.3 | 4 |
| 147 | Ranking-Oriented Quantitative Structureâ€“Activity Relationship Modeling Combined with Assay-Wise Data Integration. ACS Omega, 2021, 6, 11964-11973. | 1.6 | 4 |
| 148 | Development of a New Feed-Forward Control Method Based on Soft Sensors and Inverse Analysis. Kagaku Kogaku Ronbunshu, 2015, 41, 29-37. | 0.1 | 4 |
| 149 | Development of Soft Sensor Methods Based on Wavelength Region Selection Methods. Journal of Computer Chemistry Japan, 2012, 11, 31-42. | 0.0 | 4 |
| 150 | Development of An Adaptive Soft Sensor Method Considering Prediction Confidence of Models. Journal of Computer Chemistry Japan, 2012, 11, 24-30. | 0.0 | 4 |
| 151 | Construction of Long-Term Transmembrane Pressure Estimation Model for a Membrane Bioreactor. Journal of Computer Aided Chemistry, 2012, 13, 10-19. | 0.3 | 4 |
| 152 | Consideration of Soft Sensor Methods Based on Time Difference and Discussion on Intervals of Time Difference. Journal of Computer Aided Chemistry, 2012, 13, 29-43. | 0.3 | 4 |
| 153 | L-shaped PLS analysis of multiple inhibitory activities of adrenergic alpha receptors using ligand and protein matrices. Chemometrics and Intelligent Laboratory Systems, 2014, 130, 166-171. | 1.8 | 3 |
| 154 | Data Mining of Chemogenomics Data Using Biâ€Modal PLS Methods and Chemical Interpretation for Molecular Design. Molecular Informatics, 2014, 33, 749-756. | 1.4 | 3 |
| 155 | Application of orthogonal L-shaped PLS to chemogenomic data and its chemical interpretation from predictive and orthogonal latent variables. Chemometrics and Intelligent Laboratory Systems, 2014, 135, 166-171. | 1.8 | 3 |
| 156 | Practical Use of Savitzky-Golay Filtering-Based Ensemble Online SVR. IFAC-PapersOnLine, 2016, 49, 371-376. | 0.5 | 3 |
| 157 | Novel Electrotopological Atomic Descriptors for the Prediction of Xenobiotic Cytochrome P450 Reactions. Molecular Informatics, 2019, 38, 1900010. | 1.4 | 3 |
| 158 | Investigation of Preprocessing and Validation Methodologies for PAT: Case Study of the Granulation and Coating Steps for the Manufacturing of Ethenzamide Tablets. AAPS PharmSciTech, 2021, 22, 41. | 1.5 | 3 |
| 159 | Computer-Assisted Structure Elucidation for Organic Compound.. Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry, 1993, 51, 516-528. | 0.0 | 3 |
| 160 | Construction of a Statistical Evaluation Model Based on Molecular Centrality to Find Retrosynthetically Important Bonds in Organic Compounds. European Journal of Organic Chemistry, 2008, 2008, 5995-6007. | 1.2 | 2 |
| 161 | Application of Rule Mining to Quantative Structure-Activity Relationship Using Rough Set Theory. Journal of Computer Aided Chemistry, 2008, 9, 1-7. | 0.3 | 2 |
| 162 | Estimation of Predictive Accuracy of Soft Sensor Models Based on One-Class Support Vector Machine. Computer Aided Chemical Engineering, 2012, , 1246-1250. | 0.3 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 163 | Formulation of the excess absorption in infrared spectra by numerical decomposition for effective process monitoring. Computers and Chemical Engineering, 2018, 113, 86-97. | 2.0 | 2 |
| 164 | Metabolic disassembler for understanding and predicting the biosynthetic units of natural products. BMC Bioinformatics, 2019, 20, 728. | 1.2 | 2 |
| 165 | Improvement of the Structure Generator DAECS with Respect to Structural Diversity. Molecular Informatics, 2021, 40, 2000225. | 1.4 | 2 |
| 166 | Industrial Case Study: Identification of Important Substructures and Exploration of Monomers for the Rapid Design of Novel Network Polymers with Distributed Representation. Bulletin of the Chemical Society of Japan, 2021, 94, 112-121. | 2.0 | 2 |
| 167 | An Automatic Modeling System of the Calculation Process of a CVD Film Deposition Simulator. Journal of Chemical Engineering of Japan, 2010, 43, 977-982. | 0.3 | 2 |
| 168 | Development of a Wavelength Region Selection Method Basedon Genetic Algorithm-based WaveLength Selectionand Support Vector Regression. Journal of Computer Chemistry Japan, 2011, 10, 122-130. | 0.0 | 2 |
| 169 | Visualization and Chemical Interpretation of Multi-Target Structure-Activity Relationships Using SOMPLS. Journal of Computer Aided Chemistry, 2011, 12, 47-53. | 0.3 | 2 |
| 170 | Powerful Integrative Tool Combining Structure Generator and Chemical Space Visualization. Journal of Computer Aided Chemistry, 2012, 13, 1-9. | 0.3 | 2 |
| 171 | Improvement of Process State Recognition Performance by Noise Reduction with Smoothing Methods. Journal of Chemical Engineering of Japan, 2017, 50, 422-429. | 0.3 | 2 |
| 172 | Statistical Approach to Constructing Predictive Models for Thermal Resistance Based on Operating Conditions. Industrial & Engineering Chemistry Research, 2012, 51, 9906-9912. | 1.8 | 1 |
| 173 | Construction of Statistical Models for Predicting the Presence of Azeotropy at Any Pressure in Separation Processes. Journal of Computer Chemistry Japan, 2012, 11, 112-120. | 0.0 | 1 |
| 174 | Generative topographic mapping of binding pocket of Î²2 receptor and threeâ€way partial least squares modeling of inhibitory activities. Journal of Chemometrics, 2014, 28, 696-703. | 0.7 | 1 |
| 175 | Model for predicting transmembrane pressure jump for various membrane bioreactors. Desalination and Water Treatment, 2015, 53, 1471-1481. | 1.0 | 1 |
| 176 | Novel Method Proposing Chemical Structures with Desirable Profile of Activities Based on Chemical and Protein Spaces. Molecular Informatics, 2017, 36, 1700075. | 1.4 | 1 |
| 177 | Selective Use of Adaptive Models Considering the Prediction Efficiencies. Industrial & Engineering Chemistry Research, 2018, 57, 14286-14296. | 1.8 | 1 |
| 178 | Solubility Prediction Using Neural Network and Chemical Explanation of Deep Learning Model. Journal of Computer Aided Chemistry, 2018, 19, 1-6. | 0.3 | 1 |
| 179 | Applicability domains of a minimal-calibration model for effective online monitoring of pure componentsâ€™ concentrations in the pharmaceutical continuous manufacturing processes. Computer Aided Chemical Engineering, 2018, 44, 919-924. | 0.3 | 1 |
| 180 | Materials Informatics Approach to Predictive Models for Elastic Modulus of Polypropylene Composites Reinforced by Fillers and Additives. Journal of Computer Chemistry Japan -International Edition, 2021, 7, n/a. | 0.2 | 1 |

| # | Article | IF | Citations |
|---|---|---|---|
| 181 | Dry Etching Damage and Alloy Composition Analysis of GaN-Based Semiconductors Using Electron Energy-Loss Spectroscopy. Journal of Electronic Materials, 2021, 50, 4230-4237. | 1.0 | 1 |
| 182 | Development of a Model Predicting Transmembrane Pressurein Membrane Bioreactors. Journal of Computer Chemistry Japan, 2011, 10, 131-140. | 0.0 | 1 |
| 183 | Development of a Strategic Parameter Search Method forEfficient Product Design. Journal of Computer Chemistry Japan, 2013, 12, 113-121. | 0.0 | 1 |
| 184 | Advanced PLS Technique Focusing on Visualization and Chemical Interpretation - SOMPLS Analysis of Serine Protease Inhibitors -. Journal of Computer Aided Chemistry, 2010, 11, 56-61. | 0.3 | 1 |
| 185 | Technique of Augmenting Molecular Graph Data by Perturbating Hidden Features. Molecular Informatics, 2022, 41, . | 1.4 | 1 |
| 186 | Role of knowledge base derived from reaction database in organic synthesis design system -AIPHOS-. AIP Conference Proceedings, 1995, , . | 0.3 | 0 |
| 187 | Automatic Reaction Modeling in Chemical Vapor Depositions Using Multiple Process Simulators. Materials Research Society Symposia Proceedings, 2003, 804, 25. | 0.1 | 0 |
| 188 | An Autonomous and Intelligent System Using Mobile-Agent Software to Model the Calculation Processes of Film Deposition Simulators. Materials Research Society Symposia Proceedings, 2007, 1024, 1. | 0.1 | 0 |
| 189 | Improvement and Estimation of Prediction Accuracy of Soft Sensor Models Based on Time Difference. Lecture Notes in Computer Science, 2011, , 115-124. | 1.0 | 0 |
| 190 | Application of orthogonal L-shaped PLS to chemogenomics data and its chemical interpretation from predictive and orthogonal regression coefficients. Chemometrics and Intelligent Laboratory Systems, 2014, 139, 64-69. | 1.8 | 0 |
| 191 | Multivariate Analysis of Side Effects of Drug Molecules Based on Knowledge of Protein Bindings and Proteinï£¿Protein Interactions. Molecular Informatics, 2014, 33, 757-763. | 1.4 | 0 |
| 192 | Improvement of Prediction Accuracy in Just-In-Time Modelling Using Distance-based Database Update. Journal of Computer Aided Chemistry, 2015, 16, 1-14. | 0.3 | 0 |
| 193 | Analysis of a transmembrane pressure (TMP) jump prediction model for preventing TMP jumps. Desalination and Water Treatment, 2015, 55, 3241-3246. | 1.0 | 0 |
| 194 | Soft Sensors: Chemoinformatic Model for Efficient Control and Operation in Chemical Plants. Molecular Informatics, 2016, 35, 549-554. | 1.4 | 0 |
| 195 | Data Visualization & Clustering: Generative Topographic Mapping Similarity Assessment Allied to Graph Theory Clustering. ACS Symposium Series, 2016, , 175-210. | 0.5 | 0 |
| 196 | Improvement of Prediction Errors Based on Standardized Infrared Spectra for a Calibration-free Approach. MATEC Web of Conferences, 2021, 333, 06001. | 0.1 | 0 |
| 197 | Development of Nonlinear Soft Sensor Methods Considering Process Dynamics. Transactions of the Society of Instrument and Control Engineers, 2013, 49, 206-213. | 0.1 | 0 |
| 198 | Integration and utilization of risk information of chemical substances. Journal of Information Processing and Management, 2015, 58, 12-19. | 0.0 | 0 |

| # | Article | IF | Citations |
|---|---|---|---|
| 199 | Data Mining of Chemogenomics Data Using Activity Landscape and Partial Least Squares. , 2015, , 1723-1731. | | 0 |
| 200 | Development of TMP Prediction Model and TMP Jump Prediction Model in MBRs. Membrane, 2015, 40, 337-341. | 0.0 | 0 |
| 201 | Design of Aeration Patterns using TMP Prediction Model and TMP Jump Prediction Model for Energyâ€“saving MBRs. Membrane, 2016, 41, 155-159. | 0.0 | 0 |
| 202 | Soft-Sensor Modeling for Semi-Batch Chemical Process Using Limited Number of Sampling. Journal of Computer Aided Chemistry, 2019, 20, 119-132. | 0.3 | 0 |
| 203 | Governing Factors for Carbon Nanotube Dispersion in Organic Solvents Estimated by Machine Learning (Adv. Mater. Interfaces 7/2022). Advanced Materials Interfaces, 2022, 9, . | 1.9 | 0 |