Kimito Funatsu

List of Publications by Citations

199 papers	4,488 citations	31 h-index	62 g-index
209 ext. papers	5,264 ext. citations	3.4 avg, IF	5.75 L-index

#	Paper	IF	Citations
199	MassBank: a public repository for sharing mass spectral data for life sciences. *Journal of Mass Spectrometry*, **2010**, 45, 703-14	2.2	1321
198	GA strategy for variable selection in QSAR studies: GA-based PLS analysis of calcium channel antagonists. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 306-10		199
197	Rethinking drug design in the artificial intelligence era. *Nature Reviews Drug Discovery*, **2020**, 19, 353-364	64.1	179
196	Development of a new soft sensor method using independent component analysis and partial least squares. *AICHE Journal*, **2009**, 55, 87-98	3.6	118
195	Genetic algorithm-based wavelength selection method for spectral calibration. *Journal of Chemometrics*, **2011**, 25, 10-19	1.6	104
194	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	3.8	81
193	Maintenance-free soft sensor models with time difference of process variables. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 107, 312-317	3.8	74
192	GA strategy for variable selection in QSAR studies: application of GA-based region selection to a 3D-QSAR study of acetylcholinesterase inhibitors. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 112-20		69
191	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		62
190	Inverse QSPR/QSAR Analysis for Chemical Structure Generation (from y to x). *Journal of Chemical Information and Modeling*, **2016**, 56, 286-99	6.1	61
189	Applicability domains and accuracy of prediction of soft sensor models. *AICHE Journal*, **2011**, 57, 1506-1513	3.6	59
188	Application of online support vector regression for soft sensors. *AICHE Journal*, **2014**, 60, 600-612	3.6	56
187	Classification of the Degradation of Soft Sensor Models and Discussion on Adaptive Models. *AICHE Journal*, **2013**, 59, 2339-2347	3.6	56
186	Further development of structure generation in the automated structure elucidation system CHEMICS. *Journal of Chemical Information and Modeling*, **1988**, 28, 18-28	6.1	56
185	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	3.8	53
184	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		51
183	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	3.8	49

182	A Novel Approach to Retrosynthetic Analysis Using Knowledge Bases Derived from Reaction Databases. *Journal of Chemical Information and Computer Sciences*, **1999**, 39, 316-325		48
181	Novel soft sensor method for detecting completion of transition in industrial polymer processes. *Computers and Chemical Engineering*, **2011**, 35, 1135-1142	4	45
180	Development of a new regression analysis method using independent component analysis. *Journal of Chemical Information and Modeling*, **2008**, 48, 534-41	6.1	44
179	GA Strategy for Variable Selection in QSAR Studies: GA-Based Region Selection for CoMFA Modeling. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 276-282		44
178	Classification of Organic Reactions: 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		43
177	Fast optimization of hyperparameters for support vector regression models with highly predictive ability. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 142, 64-69	3.8	39
176	Applicability domain based on ensemble learning in classification and regression analyses. *Journal of Chemical Information and Modeling*, **2014**, 54, 2469-82	6.1	38
175	Exhaustive Structure Generation for Inverse-QSPR/QSAR. *Molecular Informatics*, **2010**, 29, 111-25	3.8	36
174	Computer-assisted organic synthesis design and reaction prediction system, AIPHOS. *Tetrahedron Computer Methodology*, **1988**, 1, 27-37		35
173	Ensemble locally weighted partial least squares as a just-in-time modeling method. *AICHE Journal*, **2016**, 62, 717-725	3.6	34
172	A new process variable and dynamics selection method based on a genetic algorithm-based wavelength selection method. *AICHE Journal*, **2012**, 58, 1829-1840	3.6	33
171	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	4	32
170	The Recent Trend in QSAR Modeling - Variable Selection and 3D-QSAR Methods. *Current Computer-Aided Drug Design*, **2007**, 3, 254-262	1.4	32
169	Varying resonance demands in substituent effects. Acetolysis of neophyl p-bromobenzenesulfonates. *Tetrahedron*, **1987**, 43, 307-316	2.4	32
168	Database monitoring index for adaptive soft sensors and the application to industrial process. *AICHE Journal*, **2014**, 60, 160-169	3.6	31
167	New molecular surface-based 3D-QSAR method using Kohonen neural network and 3-way PLS. *Computers & Chemistry*, **2002**, 26, 583-9		30
166	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	4	30
165	Computer-assisted structure/taste studies on sulfamates by pattern recognition methods. *Analytica Chimica Acta*, **1986**, 184, 143-149	6.6	29

164	Non-linear modeling and chemical interpretation with aid of support vector machine and regression. *Current Computer-Aided Drug Design*, **2010**, 6, 24-36	1.4	28
163	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	3.9	26
162	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		25
161	Quantitative structure--activity relationships of the synthetic substrates for elastase enzyme using nonlinear partial least squares regression. *Journal of Chemical Information and Computer Sciences*, **1996**, 36, 185-9		25
160	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		25
159	Chemography of natural product space. *Planta Medica*, **2015**, 81, 429-35	3.1	23
158	Novel canonical coding method for representation of three-dimensional structures. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 622-30		23
157	Substituent Effects. XVI. Acetolysis of 2-Phenylethyl Tosylates. *Bulletin of the Chemical Society of Japan*, **1987**, 60, 1091-1095	5.1	22
156	Nonlinear regression method with variable region selection and application to soft sensors. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 121, 26-32	3.8	21
155	Solvent Effects on the Solvolysis of Neophyl Tosylates. *Bulletin of the Chemical Society of Japan*, **1992**, 65, 46-54	5.1	21
154	Multivariate Statistical Process Control Method Including Soft Sensors for Both Early and Accurate Fault Detection. *Industrial & Engineering Chemistry Research*, **2014**, 53, 8553-8564	3.9	20
153	Ring-System-Based Exhaustive Structure Generation for Inverse-QSPR/QSAR. *Molecular Informatics*, **2014**, 33, 764-78	3.8	20
152	Nonlinear partial least squares modeling of phenyl alkylamines with the monoamine oxidase inhibitory activities. *Journal of Chemical Information and Computer Sciences*, **1996**, 36, 1025-9		20
151	Chemical-Space-Based de Novo Design Method To Generate Drug-Like Molecules. *Journal of Chemical Information and Modeling*, **2016**, 56, 1885-1893	6.1	19
150	Systematic generation of chemical structures for rational drug design based on QSAR models. *Current Computer-Aided Drug Design*, **2011**, 7, 1-9	1.4	19
149	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	4	18
148	Optimization of the Inner Relation Function of QPLS Using Genetic Algorithm. *Journal of Chemical Information and Computer Sciences*, **1997**, 37, 1115-1121		18
147	Representation of molecular configurations by CAST coding method. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1106-12		17

146	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	4.8	17
145	Development of a New De Novo Design Algorithm for Exploring Chemical Space. *Molecular Informatics*, **2014**, 33, 779-89	3.8	16
144	Criterion for evaluating the predictive ability of nonlinear regression models without cross-validation. *Journal of Chemical Information and Modeling*, **2013**, 53, 2341-8	6.1	16
143	Applicability domain of soft sensor models based on one-class support vector machine. *AICHE Journal*, **2013**, 59, 2046-2050	3.6	16
142	Application of infrared data analysis based on symbolic logic in automated structure elucidation by chemics. *Analytica Chimica Acta*, **1989**, 220, 155-169	6.6	16
141	Automatic recognition of reaction site in organic chemical reactions. *Tetrahedron Computer Methodology*, **1988**, 1, 53-69		16
140	Selective Use of Adaptive Soft Sensors Based on Process State. *Industrial & Engineering Chemistry Research*, **2014**, 53, 15962-15968	3.9	15
139	Combined generative topographic mapping and graph theory unsupervised approach for nonlinear fault identification. *AICHE Journal*, **2015**, 61, 1559-1571	3.6	15
138	Multi-way PLS modeling of structure-activity data by incorporating electrostatic and lipophilic potentials on molecular surface. *Computational Biology and Chemistry*, **2003**, 27, 381-6	3.6	15
137	Application of the novel molecular alignment method using the Hopfield Neural Network to 3D-QSAR. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1396-402		15
136	Substituent effect on the acetolysis of 2-phenylethyl tosylate. *Tetrahedron Letters*, **1983**, 24, 2177-2180	2	15
135	Ring system-based chemical graph generation for de novo molecular design. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 425-46	4.2	14
134	Estimation of predictive accuracy of soft sensor models based on data density. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 128, 111-117	3.8	14
133	Comparison and improvement of the predictability and interpretability with ensemble learning models in QSPR applications. *Journal of Cheminformatics*, **2020**, 12, 19	8.6	14
132	Improvement of iterative optimization technology (for process analytical technology calibration-free/minimum approach) with dimensionality reduction and wavelength selection of spectra. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 147, 176-184	3.8	13
131	Smoothing-Combined Soft Sensors for Noise Reduction and Improvement of Predictive Ability. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12630-12638	3.9	13
130	Visualization of Molecular Selectivity and Structure Generation for Selective Dopamine Inhibitors. *Molecular Informatics*, **2010**, 29, 793-800	3.8	13
129	Tailored scoring function of TrypsinBenzamidine complex using COMBINE descriptors and support vector regression. *Chemometrics and Intelligent Laboratory Systems*, **2008**, 92, 145-151	3.8	13

128	Chemoinformatics An Important Scientific Discipline. *Journal of Computer Chemistry Japan*, **2006**, 5, 53-58	0.2	13
127	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		13
126	Evolution of PLS for Modeling SAR and omics Data. *Molecular Informatics*, **2012**, 31, 766-75	3.8	12
125	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, 309-12	1.7	12
124	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		12
123	Physical and statistical model for predicting a transmembrane pressure jump for a membrane bioreactor. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 121, 66-74	3.8	11
122	Flour concentration prediction using GAPLS and GAWLS focused on data sampling issues and applicability domain. *Chemometrics and Intelligent Laboratory Systems*, **2014**, 137, 33-46	3.8	11
121	Discussion on Time Difference Models and Intervals of Time Difference for Application of Soft Sensors. *Industrial & Engineering Chemistry Research*, **2013**, 52, 1322-1334	3.9	11
120	2D and 3D QSAR studies of the receptor binding affinity of progestins. *Journal of the Brazilian Chemical Society*, **2010**, 21, 872-881	1.5	11
119	Quantitative Prediction of Regioselectivity Toward Cytochrome P450/3A4 Using Machine Learning Approaches. *Molecular Informatics*, **2010**, 29, 243-9	3.8	11
118	Novel alignment method of small molecules using the Hopfield Neural Network. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1390-5		11
117	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	3.8	10
116	Visualization of Models Predicting Transmembrane Pressure Jump for Membrane Bioreactor. *Industrial & Engineering Chemistry Research*, **2012**, 51, 9679-9686	3.9	10
115	Simultaneous determination of bioactive conformations and alignment rules by multi-way PLS modeling. *Computational Biology and Chemistry*, **2003**, 27, 211-6	3.6	10
114	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	3.4	9
113	A chemometric approach to prediction of transmembrane pressure in membrane bioreactors. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 126, 30-37	3.8	9
112	New description of protein-ligand interactions using a spherical self-organizing map. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 5410-5	3.4	9
111	Nonlinear CoMFA using QPLS as a Novel 3D-QSAR Approach. *QSAR and Combinatorial Science*, **1997**, 16, 219-223		9

110	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	1.4	9
109	Prediction of Polyethylene Density by Near-Infrared Spectroscopy Combined with Neural Network Analysis. *Journal of Computer Chemistry Japan*, **2003**, 2, 33-40	0.2	9
108	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	6.1	9
107	Random Forest Approach to QSPR Study of Fluorescence Properties Combining Quantum Chemical Descriptors and Solvent Conditions. *Journal of Fluorescence*, **2018**, 28, 695-706	2.4	8
106	Development of Drug-likeness Model and Its Visualization. *Journal of Computer Aided Chemistry*, **2008**, 9, 70-80	0.2	8
105	Bayesian Classification of Cytochrome P450 3A4 Substrates/Non-substrates and Color Mapping for Chemical Interpretation. *Journal of Computer Aided Chemistry*, **2010**, 11, 19-24	0.2	8
104	Detection of nonlinearity in soil property prediction models based on near-infrared spectroscopy. *Chemometrics and Intelligent Laboratory Systems*, **2017**, 167, 139-151	3.8	7
103	Preparation of comprehensive data from huge data sets for predictive soft sensors. *Chemometrics and Intelligent Laboratory Systems*, **2016**, 153, 75-81	3.8	7
102	Strategy of Structure Generation within Applicability Domains with One-Class Support Vector Machine. *Bulletin of the Chemical Society of Japan*, **2015**, 88, 981-988	5.1	7
101	Development of high predictive soft sensor method and the application to industrial polymer processes. *Asia-Pacific Journal of Chemical Engineering*, **2012**, 7, S39-S47	1.3	7
100	Application of data mining to quantitative structure-activity relationship using rough set theory. *Chemometrics and Intelligent Laboratory Systems*, **2009**, 99, 66-70	3.8	7
99	Advanced PLS Techniques in Chemoinformatics Studies. *Current Computer-Aided Drug Design*, **2010**, 6, 103-27	1.4	7
98	Exploring differential evolution for inverse QSAR analysis. *F1000Research*, **2017**, 6, 1285	3.6	7
97	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	4	7
96	Finding Chemical Structures Corresponding to a Set of Coordinates in Chemical Descriptor Space. *Molecular Informatics*, **2017**, 36, 1700030	3.8	6
95	Data density-based fault detection and diagnosis with nonlinearities between variables and multimodal data distributions. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 147, 58-65	3.8	6
94	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	1.6	6
93	Development of a New Index to Monitor Database for Soft Sensors. *Journal of Computer Aided Chemistry*, **2013**, 14, 11-22	0.2	6

92	Prediction of Protein?Protein Interaction Pocket Using L-Shaped PLS Approach and Its Visualizations by Generative Topographic Mapping. *Molecular Informatics*, **2014**, 33, 65-72	3.8	6
91	Automatic Determination Method Based on Cross-Validation for Optimal Intervals of Time Difference. *Journal of Chemical Engineering of Japan*, **2013**, 46, 219-225	0.8	6
90	Advanced PLS Techniques in Chemometrics and Their Applications to Molecular Design **2011**, 145-168		6
89	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	6.1	6
88	Applicability Domains and Consistent Structure Generation. *Molecular Informatics*, **2017**, 36, 1600032	3.8	5
87	Application of the mol2vec Technology to Large-size Data Visualization and Analysis. *Molecular Informatics*, **2020**, 39, e1900170	3.8	5
86	Partial constrained least squares (PCLS) and application in soft sensor. *Chemometrics and Intelligent Laboratory Systems*, **2018**, 177, 64-73	3.8	5
85	Iterative optimization technology combined with wavelength selection based on excess absorption for a process analytical technology calibration□inimum approach. *Chemometrics and Intelligent Laboratory Systems*, **2016**, 156, 137-147	3.8	5
84	Structure Modification toward Applicability Domain of a QSAR/QSPR Model Considering Activity/Property. *Molecular Informatics*, **2017**, 36, 1700076	3.8	5
83	Molecular centrality for synthetic design of convergent reactions. *Tetrahedron*, **2008**, 64, 4602-4612	2.4	5
82	Random Forest Model with Combined Features: A Practical Approach to Predict Liquid-crystalline Property. *Molecular Informatics*, **2019**, 38, e1800095	3.8	5
81	A Novel Calibration-Minimum Method for Prediction of Mole Fraction in Non-Ideal Mixture. *AAPS PharmSciTech*, **2017**, 18, 595-604	3.9	4
80	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	6.1	4
79	Classification of drug tablets using hyperspectral imaging and wavelength selection with a GAWLS method modified for classification. *International Journal of Pharmaceutics*, **2015**, 491, 130-5	6.5	4
78	Exploring Topological Pharmacophore Graphs for Scaffold Hopping. *Journal of Chemical Information and Modeling*, **2020**, 60, 2073-2081	6.1	4
77	Exploring differential evolution for inverse QSAR analysis. *F1000Research*, **2017**, 6,	3.6	4
76	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	4.2	4
75	Strategic parameter search method based on prediction errors and data density for efficient product design. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 127, 70-79	3.8	4

74	Automatic Database Monitoring for Process Control Systems. *Lecture Notes in Computer Science*, **2014**, 410-419	0.9	4
73	Application of Rough Set Theory to High Throughput Screening Data for Rational Selection of Lead Compounds. *Chem-Bio Informatics Journal*, **2008**, 8, 85-95	0.8	4
72	Core Electron Binding Energy (CEBE) as Descriptors in Quantitative Structure–Activity Relationship (QSAR) Analysis of Cytotoxicities of a Series of Simple Phenols. *QSAR and Combinatorial Science*, **2007**, 26, 378-384		4
71	Development of the computer software. *Journal of Computer Aided Chemistry*, **2005**, 6, 90-96	0.2	4
70	Development of a New Feed-Forward Control Method Based on Soft Sensors and Inverse Analysis. *Kagaku Kogaku Ronbunshu*, **2015**, 41, 29-37	0.4	4
69	Development of An Adaptive Soft Sensor Method Considering Prediction Confidence of Models. *Journal of Computer Chemistry Japan*, **2012**, 11, 24-30	0.2	4
68	Construction of Long-Term Transmembrane Pressure Estimation Model for a Membrane Bioreactor. *Journal of Computer Aided Chemistry*, **2012**, 13, 10-19	0.2	4
67	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	0.2	4
66	Development of a Novel Spectra Analysis Method to Construct Accurate NIR Models. *Journal of Computer Aided Chemistry*, **2014**, 15, 1-9	0.2	4
65	Iterative Screening Methods for Identification of Chemical Compounds with Specific Values of Various Properties. *Journal of Chemical Information and Modeling*, **2019**, 59, 2626-2641	6.1	3
64	Soft Sensor Modeling for Identifying Significant Process Variables with Time Delays. *Industrial & Engineering Chemistry Research*, **2020**, 59, 12156-12163	3.9	3
63	Process Control and Soft Sensors **2018**, 571-584		3
62	Data Mining of Chemogenomics Data Using Bi-Modal PLS Methods and Chemical Interpretation for Molecular Design. *Molecular Informatics*, **2014**, 33, 749-56	3.8	3
61	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	3.8	3
60	Practical Models for Predicting the Emission Peak Wavelengths of Inorganic Phosphors Based on Stoichiometric Information. *Chemistry Letters*, **2017**, 46, 1482-1485	1.7	3
59	A New Method for Mapping the Molecular Surface of a Protein Structure Using a Spherical Self-Organizing Map. *Molecular Informatics*, **2012**, 31, 161-6	3.8	3
58	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	5.1	3
57	Ranking-Oriented Quantitative Structure-Activity Relationship Modeling Combined with Assay-Wise Data Integration. *ACS Omega*, **2021**, 6, 11964-11973	3.9	3

56	Comparing predictive ability of QSAR/QSPR models using 2D and 3D molecular representations. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 179-193	4.2	3
55	Identification of Bioactive Scaffolds Based on QSAR Models. *Molecular Informatics*, **2018**, 37, 1700103	3.8	3
54	Formulation of the excess absorption in infrared spectra by numerical decomposition for effective process monitoring. *Computers and Chemical Engineering*, **2018**, 113, 86-97	4	2
53	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	3.8	2
52	Estimation of Predictive Accuracy of Soft Sensor Models Based on One-Class Support Vector Machine. *Computer Aided Chemical Engineering*, **2012**, 1246-1250	0.6	2
51	An Automatic Modeling System of the Calculation Process of a CVD Film Deposition Simulator. *Journal of Chemical Engineering of Japan*, **2010**, 43, 977-982	0.8	2
50	Visualization and Chemical Interpretation of Multi-Target Structure-Activity Relationships Using SOMPLS. *Journal of Computer Aided Chemistry*, **2011**, 12, 47-53	0.2	2
49	Computer-Assisted Structure Elucidation for Organic Compound.. *Yuki Gosei Kagaku Kyokaishi/Journal of Synthetic Organic Chemistry*, **1993**, 51, 516-528	0.2	2
48	Powerful Integrative Tool Combining Structure Generator and Chemical Space Visualization. *Journal of Computer Aided Chemistry*, **2012**, 13, 1-9	0.2	2
47	Metabolic disassembler for understanding and predicting the biosynthetic units of natural products. *BMC Bioinformatics*, **2019**, 20, 728	3.6	2
46	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	5.1	2
45	An Updated 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	4	2
44	Novel Electrotopological Atomic Descriptors for the Prediction of Xenobiotic Cytochrome P450 Reactions. *Molecular Informatics*, **2019**, 38, e1900010	3.8	1
43	Applicability domains of a minimal-calibration model for effective online monitoring of pure components□concentrations in the pharmaceutical continuous manufacturing processes. *Computer Aided Chemical Engineering*, **2018**, 44, 919-924	0.6	1
42	Model for predicting transmembrane pressure jump for various membrane bioreactors. *Desalination and Water Treatment*, **2015**, 53, 1471-1481		1
41	Novel Method Proposing Chemical Structures with Desirable Profile of Activities Based on Chemical and Protein Spaces. *Molecular Informatics*, **2017**, 36, 1700075	3.8	1
40	Generative topographic mapping of binding pocket of □ receptor and three-way partial least squares modeling of inhibitory activities. *Journal of Chemometrics*, **2014**, 28, 696-703	1.6	1
39	Statistical Approach to Constructing Predictive Models for Thermal Resistance Based on Operating Conditions. *Industrial & Engineering Chemistry Research*, **2012**, 51, 9906-9912	3.9	1

38	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	0.2	1
37	Application of Rule Mining to Quantative Structure-Activity Relationship Using Rough Set Theory. *Journal of Computer Aided Chemistry*, **2008**, 9, 1-7	0.2	1
36	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	3.2	1
35	Improvement of Process State Recognition Performance by Noise Reduction with Smoothing Methods. *Journal of Chemical Engineering of Japan*, **2017**, 50, 422-429	0.8	1
34	Advanced PLS Technique Focusing on Visualization and Chemical Interpretation - SOMPLS Analysis of Serine Protease Inhibitors -. *Journal of Computer Aided Chemistry*, **2010**, 11, 56-61	0.2	1
33	Ligand-based Activity Cliff Prediction Models with Applicability Domain. *Molecular Informatics*, **2020**, 39, e2000103	3.8	1
32	Practical Use of Savitzky-Golay Filtering-Based Ensemble Online SVR. *IFAC-PapersOnLine*, **2016**, 49, 371-376	0.9	1
31	Improvement of the Structure Generator DAECS with Respect to Structural Diversity. *Molecular Informatics*, **2021**, 40, e2000225	3.8	1
30	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	3.9	1
29	Selective Use of Adaptive Models Considering the Prediction Efficiencies. *Industrial & Engineering Chemistry Research*, **2018**, 57, 14286-14296	3.9	1
28	Sparse Topological Pharmacophore Graphs for Interpretable Scaffold Hopping. *Journal of Chemical Information and Modeling*, **2021**, 61, 3348-3360	6.1	1
27	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	6	1
26	Governing Factors for Carbon Nanotube Dispersion in Organic Solvents Estimated by Machine Learning. *Advanced Materials Interfaces*,2101723	4.6	0
25	Development of a Model Predicting Transmembrane Pressurein Membrane Bioreactors. *Journal of Computer Chemistry Japan*, **2011**, 10, 131-140	0.2	0
24	Development of Soft Sensor Methods Based on Wavelength Region Selection Methods. *Journal of Computer Chemistry Japan*, **2012**, 11, 31-42	0.2	0
23	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	0.2	0
22	Development of a Strategic Parameter Search Method forEfficient Product Design. *Journal of Computer Chemistry Japan*, **2013**, 12, 113-121	0.2	0
21	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	0.2	0

20	Solubility Prediction Using Neural Network and Chemical Explanation of Deep Learning Model. *Journal of Computer Aided Chemistry*, **2018**, 19, 1-6	0.2	0
19	Prediction of Reaction Yield for Buchwald-Hartwig Cross-coupling Reactions Using Deep Learning. *Molecular Informatics*, **2021**, e2100156	3.8	0
18	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	3.8	
17	Multivariate Analysis of Side Effects of Drug Molecules Based on Knowledge of Protein Bindings and Protein?Protein Interactions. *Molecular Informatics*, **2014**, 33, 757-63	3.8	
16	Improvement of Prediction Accuracy in Just-In-Time Modelling Using Distance-based Database Update. *Journal of Computer Aided Chemistry*, **2015**, 16, 1-14	0.2	
15	Analysis of a transmembrane pressure (TMP) jump prediction model for preventing TMP jumps. *Desalination and Water Treatment*, **2015**, 55, 3241-3246		
14	Improvement and Estimation of Prediction Accuracy of Soft Sensor Models Based on Time Difference. *Lecture Notes in Computer Science*, **2011**, 115-124	0.9	
13	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		
12	Automatic Reaction Modeling in Chemical Vapor Depositions Using Multiple Process Simulators. *Materials Research Society Symposia Proceedings*, **2003**, 804, 25		
11	Soft-Sensor Modeling for Semi-Batch Chemical Process Using Limited Number of Sampling. *Journal of Computer Aided Chemistry*, **2019**, 20, 119-132	0.2	
10	Integration and utilization of risk information of chemical substances. *Journal of Information Processing and Management*, **2015**, 58, 12-19		
9	Data Mining of Chemogenomics Data Using Activity Landscape and Partial Least Squares **2015**, 1723-1731		
8	Development of TMP Prediction Model and TMP Jump Prediction Model in MBRs. *Membrane*, **2015**, 40, 337-341	0	
7	Design of Aeration Patterns using TMP Prediction Model and TMP Jump Prediction Model for Energy□aving MBRs. *Membrane*, **2016**, 41, 155-159	0	
6	Development of Nonlinear Soft Sensor Methods Considering Process Dynamics. *Transactions of the Society of Instrument and Control Engineers*, **2013**, 49, 206-213	0.1	
5	Dry Etching Damage and Alloy Composition Analysis of GaN-Based Semiconductors Using Electron Energy-Loss Spectroscopy. *Journal of Electronic Materials*, **2021**, 50, 4230-4237	1.9	
4	Soft Sensors: Chemoinformatic Model for Efficient Control and Operation in Chemical Plants. *Molecular Informatics*, **2016**, 35, 549-554	3.8	
3	Data Visualization & Clustering: Generative Topographic Mapping Similarity Assessment Allied to Graph Theory Clustering. *ACS Symposium Series*, **2016**, 175-210	0.4	

2	Improvement of Prediction Errors Based on Standardized Infrared Spectra for a Calibration-free Approach. *MATEC Web of Conferences*, **2021**, 333, 06001	0.3
1	Governing Factors for Carbon Nanotube Dispersion in Organic Solvents Estimated by Machine Learning (Adv. Mater. Interfaces 7/2022). *Advanced Materials Interfaces*, **2022**, 9, 2270038	4.6