Kimito Funatsu

List of Publications by Year in Descending Order

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	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	
198	Ranking-Oriented Quantitative Structure-Activity Relationship Modeling Combined with Assay-Wise Data Integration. *ACS Omega*, **2021**, 6, 11964-11973	3.9	3
197	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	
196	Improvement of the Structure Generator DAECS with Respect to Structural Diversity. *Molecular Informatics*, **2021**, 40, e2000225	3.8	1
195	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
194	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
193	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
192	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
191	Sparse Topological Pharmacophore Graphs for Interpretable Scaffold Hopping. *Journal of Chemical Information and Modeling*, **2021**, 61, 3348-3360	6.1	1
190	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
189	Prediction of Reaction Yield for Buchwald-Hartwig Cross-coupling Reactions Using Deep Learning. *Molecular Informatics*, **2021**, e2100156	3.8	0
188	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
187	Improvement of Prediction Errors Based on Standardized Infrared Spectra for a Calibration-free Approach. *MATEC Web of Conferences*, **2021**, 333, 06001	0.3	
186	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
185	Soft Sensor Modeling for Identifying Significant Process Variables with Time Delays. *Industrial & Engineering Chemistry Research*, **2020**, 59, 12156-12163	3.9	3
184	Exploring Topological Pharmacophore Graphs for Scaffold Hopping. *Journal of Chemical Information and Modeling*, **2020**, 60, 2073-2081	6.1	4
183	Application of the mol2vec Technology to Large-size Data Visualization and Analysis. *Molecular Informatics*, **2020**, 39, e1900170	3.8	5

182	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
181	Rethinking drug design in the artificial intelligence era. *Nature Reviews Drug Discovery*, **2020**, 19, 353-364	64.1	179
180	Ligand-based Activity Cliff Prediction Models with Applicability Domain. *Molecular Informatics*, **2020**, 39, e2000103	3.8	1
179	Comparison and improvement of the predictability and interpretability with ensemble learning models in QSPR applications. *Journal of Cheminformatics*, **2020**, 12, 19	8.6	14
178	Novel Electrotopological Atomic Descriptors for the Prediction of Xenobiotic Cytochrome P450 Reactions. *Molecular Informatics*, **2019**, 38, e1900010	3.8	1
177	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
176	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
175	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
174	Soft-Sensor Modeling for Semi-Batch Chemical Process Using Limited Number of Sampling. *Journal of Computer Aided Chemistry*, **2019**, 20, 119-132	0.2	
173	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
172	Metabolic disassembler for understanding and predicting the biosynthetic units of natural products. *BMC Bioinformatics*, **2019**, 20, 728	3.6	2
171	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
170	Random Forest Model with Combined Features: A Practical Approach to Predict Liquid-crystalline Property. *Molecular Informatics*, **2019**, 38, e1800095	3.8	5
169	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
168	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
167	Process Control and Soft Sensors **2018**, 571-584		3
166	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
165	Partial constrained least squares (PCLS) and application in soft sensor. *Chemometrics and Intelligent Laboratory Systems*, **2018**, 177, 64-73	3.8	5

164	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
163	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
162	Identification of Bioactive Scaffolds Based on QSAR Models. *Molecular Informatics*, **2018**, 37, 1700103	3.8	3
161	Selective Use of Adaptive Models Considering the Prediction Efficiencies. *Industrial & Engineering Chemistry Research*, **2018**, 57, 14286-14296	3.9	1
160	Solubility Prediction Using Neural Network and Chemical Explanation of Deep Learning Model. *Journal of Computer Aided Chemistry*, **2018**, 19, 1-6	0.2	0
159	A Novel Calibration-Minimum Method for Prediction of Mole Fraction in Non-Ideal Mixture. *AAPS PharmSciTech*, **2017**, 18, 595-604	3.9	4
158	Applicability Domains and Consistent Structure Generation. *Molecular Informatics*, **2017**, 36, 1600032	3.8	5
157	Finding Chemical Structures Corresponding to a Set of Coordinates in Chemical Descriptor Space. *Molecular Informatics*, **2017**, 36, 1700030	3.8	6
156	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
155	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	3.9	9
154	Exploring differential evolution for inverse QSAR analysis. *F1000Research*, **2017**, 6,	3.6	4
153	Novel Method Proposing Chemical Structures with Desirable Profile of Activities Based on Chemical and Protein Spaces. *Molecular Informatics*, **2017**, 36, 1700075	3.8	1
152	Practical Models for Predicting the Emission Peak Wavelengths of Inorganic Phosphors Based on Stoichiometric Information. *Chemistry Letters*, **2017**, 46, 1482-1485	1.7	3
151	Structure Modification toward Applicability Domain of a QSAR/QSPR Model Considering Activity/Property. *Molecular Informatics*, **2017**, 36, 1700076	3.8	5
150	Exploring differential evolution for inverse QSAR analysis. *F1000Research*, **2017**, 6, 1285	3.6	7
149	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
148	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
147	Iterative optimization technology combined with wavelength selection based on excess absorption for a process analytical technology calibration minimum approach. *Chemometrics and Intelligent Laboratory Systems*, **2016**, 156, 137-147	3.8	5

146	Ring system-based chemical graph generation for de novo molecular design. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 425-46	4.2	14
145	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
144	Preparation of comprehensive data from huge data sets for predictive soft sensors. *Chemometrics and Intelligent Laboratory Systems*, **2016**, 153, 75-81	3.8	7
143	Design of Aeration Patterns using TMP Prediction Model and TMP Jump Prediction Model for Energy□aving MBRs. *Membrane*, **2016**, 41, 155-159	0	
142	Soft Sensors: Chemoinformatic Model for Efficient Control and Operation in Chemical Plants. *Molecular Informatics*, **2016**, 35, 549-554	3.8	
141	Ensemble locally weighted partial least squares as a just-in-time modeling method. *AICHE Journal*, **2016**, 62, 717-725	3.6	34
140	Data Visualization & Clustering: Generative Topographic Mapping Similarity Assessment Allied to Graph Theory Clustering. *ACS Symposium Series*, **2016**, 175-210	0.4	
139	Practical Use of Savitzky-Golay Filtering-Based Ensemble Online SVR. *IFAC-PapersOnLine*, **2016**, 49, 371-376	0.6	1
138	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
137	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
136	Chemography of natural product space. *Planta Medica*, **2015**, 81, 429-35	3.1	23
135	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
134	Model for predicting transmembrane pressure jump for various membrane bioreactors. *Desalination and Water Treatment*, **2015**, 53, 1471-1481		1
133	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
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	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	
130	Analysis of a transmembrane pressure (TMP) jump prediction model for preventing TMP jumps. *Desalination and Water Treatment*, **2015**, 55, 3241-3246		
129	Smoothing-Combined Soft Sensors for Noise Reduction and Improvement of Predictive Ability. *Industrial & Engineering Chemistry Research*, **2015**, 54, 12630-12638	3.9	13

128	Combined generative topographic mapping and graph theory unsupervised approach for nonlinear fault identification. *AICHE Journal*, **2015**, 61, 1559-1571	3.6	15
127	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
126	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
125	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
124	Integration and utilization of risk information of chemical substances. *Journal of Information Processing and Management*, **2015**, 58, 12-19		
123	Data Mining of Chemogenomics Data Using Activity Landscape and Partial Least Squares **2015**, 1723-1731		
122	Development of TMP Prediction Model and TMP Jump Prediction Model in MBRs. *Membrane*, **2015**, 40, 337-341	0	
121	Database monitoring index for adaptive soft sensors and the application to industrial process. *AICHE Journal*, **2014**, 60, 160-169	3.6	31
120	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
119	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
118	Applicability domain based on ensemble learning in classification and regression analyses. *Journal of Chemical Information and Modeling*, **2014**, 54, 2469-82	6.1	38
117	Selective Use of Adaptive Soft Sensors Based on Process State. *Industrial & Engineering Chemistry Research*, **2014**, 53, 15962-15968	3.9	15
116	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	
115	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
114	Ring-System-Based Exhaustive Structure Generation for Inverse-QSPR/QSAR. *Molecular Informatics*, **2014**, 33, 764-78	3.8	20
113	Development of a New De Novo Design Algorithm for Exploring Chemical Space. *Molecular Informatics*, **2014**, 33, 779-89	3.8	16
112	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	
111	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

110	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
109	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
108	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
107	Application of online support vector regression for soft sensors. *AICHE Journal*, **2014**, 60, 600-612	3.6	56
106	Automatic Database Monitoring for Process Control Systems. *Lecture Notes in Computer Science*, **2014**, 410-419	0.9	4
105	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
104	Development of a Novel Spectra Analysis Method to Construct Accurate NIR Models. *Journal of Computer Aided Chemistry*, **2014**, 15, 1-9	0.2	4
103	Estimation of predictive accuracy of soft sensor models based on data density. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 128, 111-117	3.8	14
102	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
101	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
100	A chemometric approach to prediction of transmembrane pressure in membrane bioreactors. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 126, 30-37	3.8	9
99	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
98	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
97	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
96	Nonlinear regression method with variable region selection and application to soft sensors. *Chemometrics and Intelligent Laboratory Systems*, **2013**, 121, 26-32	3.8	21
95	Development of a New Index to Monitor Database for Soft Sensors. *Journal of Computer Aided Chemistry*, **2013**, 14, 11-22	0.2	6
94	Applicability domain of soft sensor models based on one-class support vector machine. *AICHE Journal*, **2013**, 59, 2046-2050	3.6	16
93	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

92	Classification of the Degradation of Soft Sensor Models and Discussion on Adaptive Models. *AICHE Journal*, **2013**, 59, 2339-2347	3.6	56
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	Development of a Strategic Parameter Search Method forEfficient Product Design. *Journal of Computer Chemistry Japan*, **2013**, 12, 113-121	0.2	0
89	Development of Nonlinear Soft Sensor Methods Considering Process Dynamics. *Transactions of the Society of Instrument and Control Engineers*, **2013**, 49, 206-213	0.1	
88	Evolution of PLS for Modeling SAR and omics Data. *Molecular Informatics*, **2012**, 31, 766-75	3.8	12
87	Statistical Approach to Constructing Predictive Models for Thermal Resistance Based on Operating Conditions. *Industrial & Engineering Chemistry Research*, **2012**, 51, 9906-9912	3.9	1
86	Visualization of Models Predicting Transmembrane Pressure Jump for Membrane Bioreactor. *Industrial & Engineering Chemistry Research*, **2012**, 51, 9679-9686	3.9	10
85	New description of protein-ligand interactions using a spherical self-organizing map. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 5410-5	3.4	9
84	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
83	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
82	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
81	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
80	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
79	Development of Soft Sensor Methods Based on Wavelength Region Selection Methods. *Journal of Computer Chemistry Japan*, **2012**, 11, 31-42	0.2	0
78	Development of An Adaptive Soft Sensor Method Considering Prediction Confidence of Models. *Journal of Computer Chemistry Japan*, **2012**, 11, 24-30	0.2	4
77	Construction of Long-Term Transmembrane Pressure Estimation Model for a Membrane Bioreactor. *Journal of Computer Aided Chemistry*, **2012**, 13, 10-19	0.2	4
76	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
75	Powerful Integrative Tool Combining Structure Generator and Chemical Space Visualization. *Journal of Computer Aided Chemistry*, **2012**, 13, 1-9	0.2	2

74	Improvement and Estimation of Prediction Accuracy of Soft Sensor Models Based on Time Difference. *Lecture Notes in Computer Science*, **2011**, 115-124	0.9	
73	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
72	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
71	Applicability domains and accuracy of prediction of soft sensor models. *AICHE Journal*, **2011**, 57, 1506-1513	3.8	59
70	Genetic algorithm-based wavelength selection method for spectral calibration. *Journal of Chemometrics*, **2011**, 25, 10-19	1.6	104
69	Maintenance-free soft sensor models with time difference of process variables. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 107, 312-317	3.8	74
68	Novel soft sensor method for detecting completion of transition in industrial polymer processes. *Computers and Chemical Engineering*, **2011**, 35, 1135-1142	4	45
67	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
66	Development of a Model Predicting Transmembrane Pressurein Membrane Bioreactors. *Journal of Computer Chemistry Japan*, **2011**, 10, 131-140	0.2	0
65	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
64	Visualization and Chemical Interpretation of Multi-Target Structure-Activity Relationships Using SOMPLS. *Journal of Computer Aided Chemistry*, **2011**, 12, 47-53	0.2	2
63	Advanced PLS Techniques in Chemometrics and Their Applications to Molecular Design **2011**, 145-168		6
62	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
61	Advanced PLS Techniques in Chemoinformatics Studies. *Current Computer-Aided Drug Design*, **2010**, 6, 103-27	1.4	7
60	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
59	MassBank: a public repository for sharing mass spectral data for life sciences. *Journal of Mass Spectrometry*, **2010**, 45, 703-14	2.2	1321
58	Exhaustive Structure Generation for Inverse-QSPR/QSAR. *Molecular Informatics*, **2010**, 29, 111-25	3.8	36
57	Quantitative Prediction of Regioselectivity Toward Cytochrome P450/3A4 Using Machine Learning Approaches. *Molecular Informatics*, **2010**, 29, 243-9	3.8	11

56	Visualization of Molecular Selectivity and Structure Generation for Selective Dopamine Inhibitors. *Molecular Informatics*, **2010**, 29, 793-800	3.8	13
55	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
54	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
53	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
52	Development of a new soft sensor method using independent component analysis and partial least squares. *AICHE Journal*, **2009**, 55, 87-98	3.6	118
51	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
50	Development of a new regression analysis method using independent component analysis. *Journal of Chemical Information and Modeling*, **2008**, 48, 534-41	6.1	44
49	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
48	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
47	Development of Drug-likeness Model and Its Visualization. *Journal of Computer Aided Chemistry*, **2008**, 9, 70-80	0.2	8
46	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
45	Tailored scoring function of Trypsin–benzamidine complex using COMBINE descriptors and support vector regression. *Chemometrics and Intelligent Laboratory Systems*, **2008**, 92, 145-151	3.8	13
44	Molecular centrality for synthetic design of convergent reactions. *Tetrahedron*, **2008**, 64, 4602-4612	2.4	5
43	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
42	The Recent Trend in QSAR Modeling - Variable Selection and 3D-QSAR Methods. *Current Computer-Aided Drug Design*, **2007**, 3, 254-262	1.4	32
41	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		
40	Chemoinformatics – An Important Scientific Discipline. *Journal of Computer Chemistry Japan*, **2006**, 5, 53-58	0.2	13
39	Development of the computer software. *Journal of Computer Aided Chemistry*, **2005**, 6, 90-96	0.2	4

38	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
37	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
36	Simultaneous determination of bioactive conformations and alignment rules by multi-way PLS modeling. *Computational Biology and Chemistry*, **2003**, 27, 211-6	3.6	10
35	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
34	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
33	Novel alignment method of small molecules using the Hopfield Neural Network. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 1390-5		11
32	Automatic Reaction Modeling in Chemical Vapor Depositions Using Multiple Process Simulators. *Materials Research Society Symposia Proceedings*, **2003**, 804, 25		
31	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
30	New molecular surface-based 3D-QSAR method using Kohonen neural network and 3-way PLS. *Computers & Chemistry*, **2002**, 26, 583-9		30
29	Representation of molecular configurations by CAST coding method. *Journal of Chemical Information and Computer Sciences*, **2001**, 41, 1106-12		17
28	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
27	Novel canonical coding method for representation of three-dimensional structures. *Journal of Chemical Information and Computer Sciences*, **2000**, 40, 622-30		23
26	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
25	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
24	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
23	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
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21	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

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