ARAKAWA Masamoto

Organization	Business Administration
Position	Associate Professor
Academic Title	Doctor(Engineering)
Research Fields	Chemoinformatics, Information engineering, Data analysis

<< Research Subjects >>

1. Statistical data analysis
2. Efficiency of markets
3. Application of artificial intelligence

<< Academic Activities >>

Papers and Notes

1. T. Takahashi, M. Arakawa, K. Funatsu, Y. Ema, An autonomous and intelligent modeling system of the calculation process of a CVD film deposition simulator., Journal of chemical engineering of Japan, 43, 977-982 (2010)
2. M. Arakawa, Y. Yamashita, K. Funatsu, Genetic Algorithm-based Wavelength Selection Method for Spectral Calibration, Journal of chemometrics, 25, 10-19 (2011)
3. M. Arakawa, T. Miyao, K. Funatsu, Systematic Generation of Chemical Structures for Rational Drug Design based on QSAR models, Current Computer-Aided Drug Design, 7, 1-9 (2011)
4. H. Kaneko, M. Arakawa, K. Funatsu, Applicability Domains and Accuracy of Prediction of Soft Sensor Models, AIChE Journal, in press
5. H. Kaneko, M. Arakawa, K. Funatsu, Novel Soft Sensor Method for Detecting Completion of Transition in Industrial Polymer Processes, Computers & Chemical Engineering, in press
6. K. Hasegawa, M. Arakawa, K. Funatsu:"Simultaneous determination of bioactive conformations and alignment rules by multi-way PLS modeling.", Computational Biology and Chemistry, 27, 211-216 (2003)
7. H. Kaneko, M. Arakawa, K. Funatsu:"Development of a new soft sensor method using independent component analysis and partial least squares", AIChE Journal, 55, 87-98 (2009).
8. K. Hasegawa, S. Matsuoka, M. Arakawa, K. Funatsu:"Multi-way PLS modeling of structure-activity data by incorporating electrostatic and lipophilic potentials on molecular surface.", Computational Biology and Chemistry, 27, 381-386 (2003)
9. T. Miyao, M. Arakawa, K. Funatsu:"Exhaustive Structure Generation for Inverse-QSPR/QSAR", Molecular Informatics, Molecular Informatics, 29, 111-125 (2010).
10. M. Arakawa, K. Hasegawa, K. Funatsu:"Novel alignment method of small molecules using Hopfield Neural Network.", J. Chem. Inf. Comput. Sci, 43(5), 1390-1395 (2003)
11. L. S. Veras, M. Arakawa, K. Funatsu, Y. Takahata :"2D and 3D QSAR studies of the Receptor Binding Affinity of Progestins", Journal of the Brazilian Chemical Society, 21, 872-881 (2010).
12. K. Hasegawa, M. Koyama, M. Arakawa, K. Funatsu:"Application of data mining to quantitative structure-activity relationship using rough set theory", Chemom. Intell. Lab. Syst., 99, 66-70 (2009).
13. H. Kaneko, M. Arakawa, K. Funatsu:"Development of a New Regression Analysis Method Using Independent Component Analysis", J. Chem. Inf. Modell., 48(3), 534 -541 (2008).
14. M. Arakawa, K. Hasegawa, K. Funatsu:"Tailored Scoring Function of Trypsin - Benzamidine Complex Using COMBINE Descriptors and Support Vector Regression.", Chemom. Intell. Lab. Syst., 92, 145-151 (2008).
15. M. Koyama, K. Hasegawa, M. Arakawa, K. Funatsu:"Application of Rough Set Theory to High Throughput Screening Data for Rational Selection of Lead Compounds" , Chem-Bio Informatics Journal, 8, 85-95 (2008).
16. M. Arakawa, K. Hasegawa, K. Funatsu:"The recent trend in QSAR modeling - variable selection and 3D-QSAR methods.", Current Computer-Aided Drug Design, 3, 254-262 (2007).
17. Y. Takahata, M. Arakawa, K. Funatsu,M. C. A. Costa, M. Segala:"Core Electron Binding Energy (CEBE) as Descriptors in Quantitative Structure-Activity Relationship (QSAR) Analysis of Cytotoxicities of a Series of Simple Phenols.", QSAR &

Combinatorial Science, 26, 378-384 (2007).
18. M. Arakawa, K. Hasegawa, K. Funatsu:"QSAR study of anti-HIV HEPT analogues based on multi-objective genetic programming and counter-propagation neural network", Chemom. Intell. Lab. Syst., 83, 91-98 (2006).
19. K. Hasegawa, M. Arakawa, K. Funatsu:"Novel Computational Approaches in QSAR and Molecular Design Based on GA", Multi-way PLS and NN, Current Computer-Aided Drug Design, 1, 129-145 (2005).
20. M. Arakawa, K. Hasegawa, K. Funatsu:"Application of novel molecular alignment method using Hopfield Neural Network to 3D-QSAR.", J. Chem. Inf. Comput. Sci, 43(5), 1396-1402 (2003)
21. K. Hasegawa, S. Matsuoka, M. Arakawa, K. Funatsu:"New molecular surface-based 3D-QSAR method using kohonen neural network and 3-way PLS.", Computers and Chemistry, 26, 583-589 (2002).
22. K. Hasegawa, M. Arakawa, K. Funatsu:"Rational choice of bioactive conformations through use of conformation analysis and 3-way partial least squares modeling.", Chemom. Intell. Lab. Syst., 50, 253-261 (2000).
23. K. Hasegawa, M. Arakawa, K. Funatsu:"3D-QSAR study of insecticidal neonicotinoid compounds based on 3-way partial least squares model.", Chemom. Intell. Lab. Syst., 47, 33-40 (1999).

Presentations

1. M. Koyama, M. Arakawa, K. Funatsu, DEVEPOLEMENT OF THE METHOD FOR PREDICTING METABOLITES BY USING CHEMOINFORMATICS METHOD, MATH/CHEM/COMP 2009, June 8-13, 2009
2. H. Kaneko, M. Arakawa, K. Funatsu, A Novel Soft Sensor Method Detecting Completion of Transition for Industrial Polymer Processes, The 2nd IFAC International Conference on Intelligent Control Systems and Signal Processing, September 21-23, 2009
3. H. Kaneko, M. Arakawa, K. Funatsu, Approach to deterioration of prediction accuracy for practical soft sensors, The 5th International Symposium on Design, Operation and Control of Chemical Processes, 2010, July 25-28, 2010
4. S. Miki, H. Kamahara, M. Arakawa, K. Funatsu, N. Goto, A STUDY ON ESTIMATION OF MIXED CONSTRUCTION WASTES, Twelfth International Summer Symposium, JSCE, Sept. 18, 2010
5. M. Arakawa, T. Miyao, K. Funatsu:"Development and visualization of the drug-likeness model", 8th ICCS, 2008, June 1-5, 2008, Noordwijkerhout, The Netherlands
6. S. Goto, M. Arakawa, K. Funatsu:"Reverse analysis and multi-objective optimization of predictive models for polymer properties", 8th ICCS, 2008, June 1-5, 2008, Noordwijkerhout, The Netherlands
7. H. Kaneko, M. Arakawa, K. Funatsu:"Development of a new regression analysis method using independent component analysis", 8th ICCS, 2008, June 1-5, 2008, Noordwijkerhout, The Netherlands
8. M. Koyama, M. Arakawa, K. Funatsu:"Rule Induction of the site of metabolism by human Cytochromes P450 by data-mining", 8th ICCS, 2008, June 1-5, 2008, Noordwijkerhout, The Netherlands
9. T. Takahashi, N. Fukui, M. Arakawa, K. Funatsu, Y. Ema:"An Autonomous and Intelligent System Using Mobile-Agent Software to Model the Calculation Processes of Film Deposition Simulators", 2007 MRS Fall Meeting, November 26-30, 2007, Boston, MA
10. K. Funatsu, M. Arakawa:"Application of novel molecular alignment method using Hopfield neural network to 3D-QSAR", The 226th ACS National Meeting, New York, NY, September 7-11, 2003
11. K. Funatsu, M. Arakawa:"Novel Alignment method of Small Molecules Using Hopfield Neural Network", EURO-QSAR 2002, Bournemouth, UK