

John H. Kalivas Publications

J.H. Kalivas, B.R. Kowalski: "Generalized Standard Addition Method for Multicomponent Instrument Characterization and Elimination of Interferences in Inductively Coupled Plasma Spectrometry", *Analytical Chemistry*, **53**, 2207-2212 (1981).

J.H. Kalivas, B.R. Kowalski: "Compensation for Drift and Interferences in Multicomponent Analysis", *Analytical Chemistry*, **54**, 560-565 (1982).

J.H. Kalivas, B.R. Kowalski: "Automated Multicomponent Analysis with Correction for Interferences and Matrix Effects", *Analytical Chemistry*, **55**, 532-535 (1983).

J.H. Kalivas: "Precision and Stability for the Generalized Standard Addition Method", *Analytical Chemistry*, **55**, 565-567 (1983).

I.E. Frank, J.H. Kalivas, B.R. Kowalski: "Partial Least Squares Solutions for Multicomponent Analysis", *Analytical Chemistry*, **55**, 1800-1804 (1983).

J.H. Kalivas: "Determination of Optimal Parameters for Multicomponent Analysis Using the Calibration Matrix Condition Number", *Analytical Chemistry*, **58**, 989-992 (1986).

L.L. Juhl, J.H. Kalivas: "Evaluation of the Calibration Matrix Condition Number As a Criterion for Optimal Derivative Spectrophotometric Multicomponent Analysis", *Analytica Chimica Acta*, **187**, 347-351 (1986).

J.H. Kalivas: "A Simplex Optimized Inductively Coupled Plasma Spectrometer with Minimization of Interferences", *Applied Spectroscopy*, **41**, 1338-1342 (1987).

J.H. Kalivas: "Evaluation of Volume and Matrix Effects for the Generalized Standard Addition Method", *Talanta*, **34**, 899-903 (1987).

L.L. Juhl, J.H. Kalivas: "Evaluation of Experimental Designs for Multicomponent Analysis with Spectrophotometry", *Analytica Chimica Acta*, **207**, 125-135 (1988).

J.H. Kalivas, C.W. Blount: "Error Analysis for Multicomponent Systems", *Journal of Chemical Education*, **65**, 794-795 (1988).

J.H. Kalivas: "Variance-Decomposition of Pure-Component Spectra as a Measure of Selectivity", *Journal of Chemometrics*, **3**, 409-418 (1989).

J.H. Kalivas: "Assessing Spectral Orthogonality", *Applied Spectroscopy Reviews*, **25**, 229-259 (1989).

J.H. Kalivas, P. Lang: "Condition Numbers, Iterative Refinement and Error Bounds", *Journal of Chemometrics*, **3**, 443-449 (1989).

J.H. Kalivas, N. Roberts, J. Sutter: "Global Optimization by Simulated Annealing with Wavelength Selection for Ultraviolet-Visible Spectrophotometry", *Analytical Chemistry*, **61**, 2024-2030 (1989).

L.L. Juhl, J.H. Kalivas, J.M. Sutter: "Observations of Trends for Singular Values and Eigenvectors from Library Searching Ultraviolet/Visible Spectra with Spectral Subtraction", *Analytica Chimica Acta*, **237**, 223-232 (1990).

J.H. Kalivas: "Generalized Simulated Annealing for Calibration Sample Selection From an Existing Set and Orthogonalization of Undesigned Experiments", *Journal of Chemometrics*, **5**, 37-48 (1991).

J.M. Sutter, J.H. Kalivas: "Convergence of Generalized Simulated Annealing with Variable Step Size with Application Toward Parameter Estimations of Linear and Nonlinear Models", *Analytical Chemistry*, **63**, 2383-2386 (1991).

K. Hitchcock, J.M. Sutter, J.H. Kalivas: "Computer-Generated Multicomponent Calibration Designs for Optimal Analysis Sample Predictions", *Journal of Chemometrics*, **6**, 85-96 (1992).

T.D. Jarvis, J.H. Kalivas: "Fundamentals of Condition Index Evolving Profiles for Qualitative Analysis of Unresolved Chromatographic Peaks", *Analytica Chimica Acta*, **266**, 13-24 (1992).

J.H. Kalivas: "Optimization Using Variations of Simulated Annealing", *Chemometrics and Intelligent Laboratory Systems*, **15**, 1-12 (1992).

J.H. Kalivas: "Chemometrics with Undergraduates", *Chemometrics and Intelligent Laboratory Systems*, **15**, 127-135 (1992).

J.M. Sutter, J.H. Kalivas, P.M. Lang: "Which Principal Components to Utilize for Principal Component Regression", *Journal of Chemometrics*, **6**, 217-225 (1992).

J.H. Kalivas: "Chapter 4, Calibration" in **Practical Guide to Chemometrics**, editor S.J. Haswell, Marcel Dekker, New York , (1992).

J.H. Kalivas: "Calibration Design: Samples and Wavelengths" in **Trends in Applied Spectroscopy, Vol. 1**, editor J. Menon, Research Trends, India, 173-186 (1993).

T.D. Jarvis, J.H. Kalivas: "Condition Index Evolving Profile Library Searches: Gas Chromatography-Fourier Transform Infrared Spectrometry Application", *Analytica Chimica Acta*, **272**, 53-59 (1993).

J.M. Sutter, J.H. Kalivas: "Comparison of Forward Selection, Backward Elimination, and Generalized Simulated Annealing for Variable Selection", *Microchemical Journal*, **47**, 60-66 (1993).

P.M. Lang, J.H. Kalivas: "A Global Perspective on Multivariate Methods in Spectral Chemical Analysis", *Journal of Chemometrics*, **7**, 153-163 (1993).

J.H. Kalivas, P.M. Lang: **Mathematical Analysis of Spectral Orthogonality**, Marcel Dekker, New York , (1994).

J.H. Kalivas (editor): **Adaption of Simulated Annealing to Chemical Optimization Problems**, Elsevier, The Netherlands, (1995).

G.A. Bakken, J.H. Kalivas: "Assessing Chromatographic Peak Purity Using Condition Index and Singular Value Evolving Profiles", *Analytica Chimica Acta*, **300**, 173-181 (1995).

U. Hörchner, J.H. Kalivas: "Further Investigation on a Comparative Study of Simulated Annealing and Genetic Algorithm for Wavelength Selection", *Analytica Chimica Acta*, **311**, 1-13 (1995).

U. Hörchner, J.H. Kalivas: "Simulated Annealing Type Optimization Algorithms: Fundamentals and Wavelength Selection Applications", *Journal of Chemometrics*, **9**, 283-308 (1995).

U. Hörchner, J.H. Kalivas: "Comparison of Algorithms for Wavelength Selection" in **Adaption of Simulated Annealing to Chemical Optimization Problems**, editor J.H. Kalivas, Elsevier, The Netherlands, (1995).

G.A. Bakken, N.J. Messick, J.H. Kalivas: "Singular Value Evolving Profiles of Spectrochromatographic Data for Detection of Impurities and Determination of Component-Wise Elution Regions" in **Recent Developments in Applied Spectroscopy, Vol. 1**, editor Scientific Information Guild, Research Signpost, India, 41-51 (1996).

J.H. Kalivas, U. Hörchner: "Improved Calibrations for NIR Spectra by Wavelength Selection" in **Recent Developments in Applied Spectroscopy, Vol. 1**, editor Scientific Information Guild, Research Signpost, India, 25-39 (1996).

J.H. Kalivas, P.M. Lang: "Interrelationships Between Sensitivity and Selectivity Measures for Spectroscopic Analysis", *Chemometrics and Intelligent Laboratory Systems*, **32**, 135-149 (1996).

N.J. Messick, J.H. Kalivas, P.M. Lang: "Selectivity and Related Measures for n th-Order Data", *Analytical Chemistry*, **68**, 1572-1579 (1996).

G.A. Bakken , N.J. Messick, J.H. Kalivas: "Determination of Component-Wise Chromatographic Elution Regions Using Singular Value Evolving Profiles", *Analytica Chimica Acta*, **334**, 15-25 (1996).

N.J. Messick, J.H. Kalivas: "Determination of Chromatographic Elution Profiles Using Non-Normalized Singular Value Evolving Profiles", *Microchemical Journal*, **55**, 235-246 (1997).

N.J. Messick, J.H. Kalivas, P.M. Lang: "Selecting Factors for Partial Least Squares", *Microchemical Journal*, **55**, 200-207 (1997).

Y.L. Xie, J.H. Kalivas: "Use of Matrix Orthogonal Projection to Peak Purity Assessment", *Analytical Letters*, **30**, 395-416 (1997).

J.M. Brenchley, U. Hörcchner, J.H. Kalivas: "Wavelength Selection Characterization for NIR Spectra", *Applied Spectroscopy*, **51**, 689-699 (1997).

Y.L. Xie, J.H. Kalivas: "Evaluation of Principal Component Selection Methods to Form a Global Prediction Model by Principal Component Regression", *Analytica Chimica Acta*, **348**, 19-27 (1997).

Y.L. Xie, J.H. Kalivas: "Local Prediction Models by Principal Component Regression", *Analytica Chimica Acta*, **348**, 29-38 (1997).

J.H. Kalivas, P.M. Lang: "Response to "Comments on Interrelationships Between Sensitivity and Selectivity Measures for Spectroscopic Analysis""", *Chemometrics and Intelligent Laboratory Systems*, **38**, 95-100 (1997).

J.H. Kalivas: "Two Data Sets of Near Infrared Spectra", *Chemometrics and Intelligent Laboratory Systems*, **37**, 255-259 (1997).

G.A. Bakken, D.R. Long, J.H. Kalivas, "Examination of Criteria for Local Model Principal Component Regression", *Applied Spectroscopy*, **51**, 1814-1822 (1997).

P.M. Lang, J.M. Brenchley, R.G. Nieves, J.H. Kalivas, "Cyclic Subspace Regression", *Journal of Multivariate Analysis*, **65**, 58-70 (1998).

J.M. Brenchley, R.G. Nieves, P.M. Lang, J.H. Kalivas, "Stabilization of Cyclic Subspace Regression", *Chemometrics and Intelligent Laboratory Systems*, **41**, 127-134 (1998).

C.E. Anderson, R.G. Nieves, J.H. Kalivas, "Spectral Orthogonality Considerations for Library Searching N th-Order Data", *Chemometrics and Intelligent Laboratory Systems*, **41**, 115-125 (1998).

J.H. Kalivas, "Cyclic Subspace Regression with Analysis of the Hat Matrix", *Chemometrics and Intelligent Laboratory Systems*, **45**, 209-217 (1998).

G.A. Bakken, T.P. Houghton, J.H. Kalivas, "Cyclic Subspace Regression with Analysis of Wavelength Selection Criteria", *Chemometrics and Intelligent Laboratory Systems*, **45**, 219-232 (1998).

J.H. Kalivas, "Interrelationships of Multivariate Regression Methods Using Eigenvector Basis Sets", *Journal of Chemometrics*, **13**, 111-132 (1999).

V.A. Allen, J.H. Kalivas, R.G. Rodriguez, "Post-Consumer Plastic Identification Using Raman Spectroscopy", *Applied Spectroscopy*, **53**, 672-681 (1999).

C.E. Anderson, J.H. Kalivas, "Fundamentals of Calibration Transfer Through Procrustes Analysis", *Applied Spectroscopy*, **53**, 1268-1276 (1999).

J.J. Rosentreter, R. Nieves, J. Kalivas, J. Rousseau, R.C. Bartholomay, "The Use of Chemical and Physical Properties for Rapid Characterization of Strontium Distribution Coefficients at the Idaho National Engineering and Environmental Laboratory, Idaho ", U.S. Geological Survey, Water Resources Investigations Report, 99-4123 (June 1999).

T. Houghton, J.H. Kalivas, "Implementation of Traditional and Real-World Cooperative Learning Techniques in Quantitative Analysis Including Near Infrared Spectroscopy for Analysis of Live Trout", *Journal of Chemical Education*, **77**, 1314-1318 (2000).

J.M. Brenchley, R.L. Green, S.Z. Fairchild, J.H. Kalivas, G. Scalarone, "Capability of Urine Analysis for the Disease Blastomycosis Using Infrared Spectroscopy with Eigenvector Signal to Noise Assessment", *Analytical Letters*, **33**, 3165-3181 (2000).

S.Z. Fairchild, J.H. Kalivas, "PCR Eigenvector Selection Based on Correlation Relative Standard Deviations", *Journal of Chemometrics*, **15**, 615-625 (2001).

J.H. Kalivas, R.L. Green, "Pareto Optimal Multivariate Calibration for Spectroscopic Data", *Applied Spectroscopy*, **55**, 1645-1652 (2001).

J. H. Kalivas, "Basis Sets for Multivariate Calibration", *Analytica Chimica Acta*, **428**, 31-40 (2001).

R. L. Green, J. H. Kalivas, "Graphical Diagnostics for Regression Model Determinations with Consideration of the Bias/Variance Trade-off", *Chemometrics and Intelligent Laboratory Systems*, **60**, 173-188 (2002).

N.M. Faber, J. Ferre, R. Boque, J.H. Kalivas, "Second-order Bilinear Calibration: The Effects of Vectorising the Data Matrices of the Calibration Set", *Chemometrics and Intelligent Laboratory Systems*, **63**, 107-116 (2002).

K.J. Anderson, J.H. Kalivas, "Assessment of Pareto Calibration, Stability, and Wavelength Selection", *Applied Spectroscopy*, **57**, 309-316 (2003).

J.M. Clark, K.A. Daum, J.H. Kalivas, "Demonstrated Potential of Ion Mobility Spectrometry for Detection of Adulterated Perfumes and Plant Speciation", *Analytical Letters*, **36**, 215-244 (2003).

N.M. Faber, J. Ferré, R. Boqué, J.H. Kalivas, "Quantifying Selectivity in Spectrophotometric Multicomponent Analysis", *Trends in Analytical Chemistry*, **22**, 352-361 (2003).

J.H. Kalivas, "Pareto Calibration with Built-in Wavelength Selection", *Analytica Chimica Acta*, **505**, 9-14 (2004).

J.H. Kalivas, J.B. Forrester, H.A. Seipel, "QSAR Modeling Based on the Bias/Variance Compromise: A Harmonious Approach", *Journal of Computer-Aided Molecular Design*, **18**, 537-547 (2004).

H.A. Seipel, J.H. Kalivas, "Effective Rank for Multivariate Calibration Methods", *Journal of Chemometrics*, **18**, 306-311 (2004).

J.B. Forrester, J.H. Kalivas, "Ridge Regression Optimization Using a Harmonious Approach", *Journal of Chemometrics*, **18**, 372-384 (2004).

J.H. Kalivas, "Realizing Work Place Skills in Instrumental Analysis", *Journal of Chemical Education*, **82**, 895-3897, (2005).

J.H. Kalivas, "Multivariate Calibration: An Overview", *Analytical Letters*, **38**, 2259-2279 (2005).

A.C. Olivieri, N.M. Faber, J. Ferr, R. Boque, J.H. Kalivas, H. Mark: "Uncertainty Estimation and Figures of Merit for Multivariate Calibration", *Pure and Applied Chemistry*, **78**, 633-661 (2006).

P.J. Gemperline, J.H. Kalivas: " Chapter 3, Sampling Theory, Distribution Functions and the Multivariate Normal Distribution" in **Practical Guide to Chemometrics, Second Edition**, editor

P.J. Gemperline, CRC Press Taylor & Francis Group, Boca Raton, Florida (2006).

J.H. Kalivas, P.J. Gemperline: " Chapter 5, Calibration" in **Practical Guide to Chemometrics, Second Edition**, editor P.J. Gemperline, CRC Press Taylor & Francis Group, Boca Raton, Florida (2006).

F. Stout, J.H. Kalivas: "Tikhonov Regularization in Standard and General Form for Multivariate Calibration with Applications Towards Removing Unwanted Spectral Artifacts", *Journal of Chemometrics*, **20**, 22-33 (2006).

F. Stout, M.R. Baines, J.H. Kalivas: "Impartial Graphical Comparison of Multivariate Calibration Methods and the Harmony/Parsimony Tradeoff", *Journal of Chemometrics*, **20**, 464-475 (2006).

F. Stout, J.H. Kalivas, K. Heberger: "Wavelength Selection for Multivariate Calibration Using Tikhonov Regularization", *Applied Spectroscopy*, **61**, 85-95 (2007).

J.H. Kalivas: "Progression of Chemometrics in Research Supportive Curricula" in *Active Learning: Models from the Analytical Sciences, ACS Symposium Series 970*, editor P.A. Mabrouk, Oxford University Press, (2007).

F. Stout, J.H. Kalivas: "Evaluation of Multivariate Calibration Using a Tikhonov Regularization Approach and the Generalized Pair-Correlation Method with Non-linear Data", *Analytical Letters*, **40**, 1227-1251 (2007).

J.H. Kalivas: "Learning from Procrustes Analysis to Improve Multivariate Calibration", *Journal of Chemometrics*, **22**, 227-234 (2008).

O. Farkas, I.G. Zenkevich, F. Stout, J.H. Kalivas, K. Heberger: "Prediction of Gas Chromatographic Retention Indices for Fatty Acid Methyl Esters", *Journal Chromatography A*, **1198-1199**, 188-195 (2008).

J.H. Kalivas: "An Elementary School Service Learning Project Based on a Research Supportive Curriculum Format in the General Chemistry Laboratory", *Journal of Chemical Education*, **85**, 1410-1415 (2008).

J.H. Kalivas (section editor): "Linear Regression Modeling" in **Comprehensive Chemometrics: Chemical and Biochemical Data Analysis**, editors-in-chief S. Brown, R. Tauler, and B. Walczak, Elsevier, The Netherlands, (2009).

J.H. Kalivas: "Methodologies" in **Comprehensive Chemometrics: Chemical and Biochemical Data Analysis**, editors-in-chief S. Brown, R. Tauler, and B. Walczak, Elsevier, The Netherlands, (2009).

J.H. Kalivas, G.G. Siano, E. Andries, H.C. Goicoechea: "Calibration Maintenance and Transfer Using Tikhonov Regularization Approaches", *Applied Spectroscopy*, **63**, 800-809 (2009)

M.R. Kunz, J. Ottaway, J.H. Kalivas, E. Andries: "Impact of Standardization Sample Designs on Tikhonov Regularization Variants for Spectroscopic Calibration and Maintenance and Transfer", *Journal of Chemometrics*, **24**, 218-229 (2010).

E. Andries, J.H. Kalivas, "Multivariate Calibration Leverages and Spectral F-Ratios via the Filter Factor Representation", *Journal of Chemometrics*, **24**, 249-260 (2010).

R. Kunz, J.H. Kalivas, E. Andries: "Model Updating for Spectral Calibration Maintenance and Transfer Using 1-Norm Variants of Tikhonov Regularization", *Analytical Chemistry*, **82**, 3642-3649 (2010).

J. Ottaway, J.H. Kalivas, E. Andries: "Spectral Multivariate Calibration with Wavelength Selection Using Variants of Tikhonov Regularization", *Applied Spectroscopy*, **64**, 1388-1395 (2010).

M.R. Kunz, J. Ottaway, J.H. Kalivas, C.A. Georgiou, G.A. Mousdis: "Updating a Synchronous Fluorescence Spectroscopic Virgin Olive Oil Adulteration Calibration to a New Geographical Region", *Journal of Agricultural and Food Chemistry*, **59**, 1051-1057 (2011).

J. Farrell, K. Higgins, J.H. Kalivas: "Updating a Near-Infrared Multivariate Calibration Model Formed with Lab-Prepared Pharmaceutical Tablet Types to New Tablet Types in Full Production", *Journal of Pharmaceutical and Biomedical Analysis*, **61**, 114-121 (2012).

K. Higgins, J.H. Kalivas, E. Andries: "Evaluation of Target Factor Analysis and Net Analyte Signal as Processes for Classification Purposes with Application to Benchmark Data Sets and Extra Virgin Olive Oil Adulteration", *Journal of Chemometrics*, **26**, 66-75 (2012).

J.H. Kalivas: "Overview of Two-norm (L2) and One-norm (L1) Regularization Variants for Full Wavelength or Sparse Spectral Multivariate Calibration Models or Maintenance", *Journal of Chemometrics*, **26**, 218-230 (2012).

P. Shahbazikhah, J.H. Kalivas: "A Consensus Modeling Approach to Update a Spectroscopic Calibration", *Chemometrics and Intelligent Laboratory Systems*, **120**, 142-153 (2013).

J. Ottaway, J. Farrell, J.H. Kalivas: "Spectral Multivariate Calibration without Laboratory Prepared or Determined Reference Analyte Values", *Analytical Chemistry*, **85**, 1509-1516 (2013).

E. Andries, J.H. Kalivas: "Interrelationships between Generalized Tikhonov Regularization, Generalized Net Analyte Signal, and Generalized Least Squares for Desensitizing a Multivariate Calibration to Interferences", *Journal of Chemometrics*, **27**, 126-140 (2013).

J.H. Kalivas, J. Palmer: "Characterizing Multivariate Calibration Tradeoffs (Bias, Variance, Selectivity, and Sensitivity) to Select Model Tuning Parameters", *Journal of Chemometrics*, **28**, 347-357 (2014).

J.H. Kalivas: "The Flexibility of Regularization Processes for Multivariate Calibration Maintenance", *European Pharmaceutical Review*, **19(4)**, 21-24 (2014).

J.H. Kalivas, C.A. Georgiou, M. Moira, I. Tsafaras, E. Petrakis, G.A. Mousdis: "Food Adulteration Analysis without Laboratory Prepared or Determined Reference Food Adulterant Values", *Food Chemistry*, **148**, 289-293 (2014). For a PowerPoint presentation, see
<https://www.sciencedirect.com/science/article/pii/S030881461301501X>

S.A. Drivelos, K. Higgins, J.H. Kalivas, S.A. Haroutounian, C.A. Georgiou: "Data Fusion for Food Authentication. Combining Rare Earth Elements and Trace Metal to Discriminate "Fava Santorinis" from Other Yellow Split Peas using Chemometric Tools", *Food Chemistry*, **165**, 316-322 (2014).

J. Ottaway, J.H. Kalivas: "Feasibility Study to Transform Spectral and Instrumental Artifacts for Multivariate Calibration Maintenance", *Applied Spectroscopy*, **69**, 407-416 (2015).

J.H. Kalivas, K. Héberger, E. Andries: "Using Sum of Ranking Differences (SRD) to Ensemble Multivariate Calibration Model Merits for Tuning Parameter Selection and Comparing Calibration Methods", *Analytica Chimica Acta*, **869**, 21-33 (2015).

J. Palmer, J.H. Kalivas: "Net Analyte Signal (NAS) for Selection of Multivariate Calibration Models and Development of NAS Sample-Wise Target Calibration Model Attributes" in **ACS Symposium, 40 Years of Chemometrics**, editor B. Lavine, Oxford University Press (2015).

P. Shahbazikhah, J.H. Kalivas, E. Andries, T. O'Loughlin: "Using the L1 Norm to Select Basis Set Vectors for Multivariate Calibration and Calibration Updating", *Journal of Chemometrics*, **30**, 109-120 (2016).

A. Tencate, J.H. Kalivas, E. Andries: "Penalty Processes for Combining Roughness and Smoothness in Spectral Multivariate Calibration", *Journal of Chemometrics*, **30**, 144-152 (2016).

A.J. Tencate, J.H. Kalivas, A.J. White: "Fusion Strategies for Selecting Multiple Tuning Parameters for Multivariate Calibration and other Penalty Based Processes: A Model Updating Application for Pharmaceutical Analysis", *Analytica Chimica Acta*, **921**, 28-37 (2016).

B. Brownfield, J.H. Kalivas: "Consensus Outlier Detection using Sum of Ranking Differences of Common and New Outlier Measures without Tuning Parameter Selections", *Analytical Chemistry*, **89**, 5087-5094 (2017) <https://doi.org/10.1021/acs.analchem.7b00637>

J.H. Kalivas, J. Ferré, A.J. Tencate: "Selectivity-Relaxed Classical and Inverse Least Squares Calibration and Selectivity Measures with a Unified Selectivity Coefficient", *Journal of Chemometrics*, **31**, 1-23 (2017) Open Access, <http://onlinelibrary.wiley.com/doi/10.1002/cem.2925/epdf>

J.H. Kalivas, B. Brownfield, B. Karki: "Sample-Wise Spectral Multivariate Calibration Desensitized to New Artifacts Relative to the Calibration Data Using a Residual Penalty", *Journal of Chemometrics*, **31**(4), 1-12 (2017) <https://doi.org/10.1002/cem.2873>.

T. Lemos, J.H. Kalivas: "Leveraging Multiple Linear Regression for Wavelength Selection", *Chemometrics and Laboratory Systems*, **168**, 121-127 (2017) <https://doi.org/10.1016/j.chemolab.2017.07.011>

T. Stokes, M. Foteini, B. Brownfield, J.H. Kalivas, G. Mousdis, A. Amine, and C. Georgiou: "Fusion of Synchronous Fluorescence Spectra with Application to Argan Oil for Adulteration Analysis", *Applied Spectroscopy*, **72**, 432-441 (2018) <https://doi.org/10.1177/0003702817749232>.

B. Brownfield, T. Lemos, J.H. Kalivas: "Consensus Classification Using Non-Optimize Classifiers", *Analytical Chemistry*, **90**, 4429-4437 (2018) <https://doi.org/10.1021/acs.analchem.7b04399>.

J.H. Kalivas: "Chapter 12: Data Fusion of Non-Optimized Models: Applications to Outlier Detection, Classification, and Image Library Searching", in **Data Fusion Methodology and Applications**, editor M. Cocchi, Elsevier, The Netherlands, (2019).

E. Andries, J.H. Kalivas, A. Gurung: "Sample and Feature Augmentation Strategies for Calibration Updating: A Comparative Study", *Journal of Chemometrics*, **33**(1), e3080, 1-20 (2019)
<https://doi.org/10.1002/cem.3080>.

I. Unobe, L. Lau, J. Kalivas, R. Rodriguez, A. Sorensen: "Restoration of Defaced Serial Numbers Using Lock-in Infrared Thermography (Part I)", *Journal of Spectral Imaging*, **8**, Article ID a19 (2019) Open Access <https://doi.org/10.1255/jsi.2019.a19>.

I. Unobe, L. Lau, J. Kalivas, R. Rodriguez, A. Sorensen: "Restoration of Defaced Serial Numbers Using Lock-in Infrared Thermography (Part II)", *Journal of Spectral Imaging*, **8**, Article ID a20 (2019) Open Access <https://doi.org/10.1255/jsi.2019.a20>.

T. Lemos, R. Emerson, J.H. Kalivas: "Identifying Chemical, Physical, and Instrumental Matrix Matched Samples by Leveraging Spectral Model Regression Vectors", *Analytical Chemistry* **92**, 815-823 (2020) <http://dx.doi.org/10.1021/acs.analchem.9b03302>.

T. Lemos, J.H. Kalivas: "Self-Optimized One-Class Classification Using Sum of Ranking Differences Combined with a Receiver Operator Characteristic Curve", *Analytical Chemistry*, **92**, 5354-5361 (2020) <http://doi.org/10.1021/acs.analchem.0c00017>.

A. Gurung, J.H. Kalivas: "Model Selection Challenges with Application to Multivariate Calibration Updating Methods", *Journal Chemometrics* 2020;e3245. <https://doi.org/10.1002/cem.3245>

B.K. Chabuka, J.H. Kalivas: "Application of a Hybrid Fusion Classification Process for Identification of Microplastics Based on FTIR Spectroscopy", *Applied Spectroscopy*, **74**, 1167-1183 (2020) <https://doi.org/10.1177/0003702820923993>.

J.H. Kalivas, S.D. Brown: "Calibration Methodologies" in **Comprehensive Chemometrics: Chemical and Biochemical Data Analysis**, 2nd Edition, editors-in-chief S. Brown, R. Tauler, and B. Walczak, Elsevier, The Netherlands, (2020) <https://doi.org/10.1016/B978-0-12-409547-2.14666-9>.

E. Struhs, S. Hansen, A. Mirkouei, M.M. Ramirez-Corredores, K. Sharma, R. Spiers, J.H. Kalivas: "Ultrasonic-Assisted Catalytic Transfer Hydrogenation for Upgrading Pyrolysis-oil", *Ultrasonics Sonochemistry*, **73**, 105502 (2021), Open Access
<https://doi.org/10.1016/j.ultsonch.2021.105502>.

R.C. Spiers, J.H. Kalivas: "Reliable Model Selection without Reference Values by Utilizing Model Diversity with Prediction Similarity", *Journal of Chemical Information and Modeling*, **61**, 2220-2230 (2021) <https://doi.org/10.1021/acs.jcim.0c01493>.

R.C. Spiers, J.H. Kalivas: "Calibration Model Updating to Novel Sample and Measurement Conditions without Reference Values", *Analytical Chemistry*, **93**, 9688-9696 (2021) <https://doi.org/10.1021/acs.analchem.1c00578>.

J.H. Kalivas, T. Lemos: "Automatic Food and Beverage Authentication and Adulteration Detection by Classification Hybrid Fusion", *Journal of Chemometrics*, **37(3)** 2023:e3371 <https://doi.org/10.1002/cem.3371>.

R.C. Spiers, C. Norby, J.H. Kalivas: "Physicochemical Responsive Integrated Similarity Measure (PRISM) for a Comprehensive Quantitative Perspective of Sample Similarity Dynamically Assessed with NIR Spectra", *Analytical Chemistry*, **95**, 12776–12784 (2023) <https://doi.org/10.1021/acs.analchem.3c01616>.

J.M.J. Peper, J.H. Kalivas: "Local Modeling by Adapting Source Calibration Models to Analyte Shifted Target Domain Samples without Reference Values", *Applied Spectroscopy*, **78**, 922-932 (2024) <https://doi.org/10.1177/00037028241241557>.

R.C. Spiers, J.H. Kalivas: "Local Adaptive Fusion Regression (LAFR) for Local Linear Multivariate Calibration: Application to Large Datasets", *Applied Spectroscopy*, **79**, 797-807 (2025) <https://doi.org/10.1177/00037028241308538>.

J.M.J. Peper, J.H. Kalivas: "Redefining Spectral Data Analysis with Immersive Analytics: Exploring Domain Shifted Model Spaces for Optimal Model Selection", *Applied Spectroscopy*, **79**, 942-954 (2025) <https://doi.org/10.1177/00037028241280669>.

H.J. Redd, J.H. Kalivas: "Assessment of Conformal Prediction and Standard Normal Distribution for Autonomous Consensus One-Class Classification", *Journal of Chemometrics*, 39:e3639 (2025) <https://doi.org/10.1002/cem.3639>.

J.H. Kalivas: "Perspective on the Capacity of the Rashomon Effect in Multivariate Data Analysis", *Applied Spectroscopy*, in press (2025) <https://doi.org/10.1177/00037028251330324>.