

# John H Kalivas

## List of Publications by Year in descending order

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85  
papers

2,647  
citations

186265  
28  
h-index

197818  
49  
g-index

89  
all docs

89  
docs citations

89  
times ranked

1814  
citing authors

| #  | ARTICLE  | IF  | CITATIONS |
|----|--|-----|-----------|
| 1  | Automatic food and beverage authentication and adulteration detection by classification hybrid fusion. <i>Journal of Chemometrics</i> , 2023, 37, e3371.                                       | 1.3 | 2         |
| 2  | Reliable Model Selection without Reference Values by Utilizing Model Diversity with Prediction Similarity. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2220-2230.          | 5.4 | 5         |
| 3  | Ultrasonic-assisted catalytic transfer hydrogenation for upgrading pyrolysis-oil. <i>Ultrasonics Sonochemistry</i> , 2021, 73, 105502.   | 8.2 | 11        |
| 4  | Calibration Model Updating to Novel Sample and Measurement Conditions without Reference Values. <i>Analytical Chemistry</i> , 2021, 93, 9688-9696.   | 6.5 | 7         |
| 5  | Identifying Chemical, Physical, and Instrumental Matrix Matched Samples by Leveraging Spectral Model Regression Vectors. <i>Analytical Chemistry</i> , 2020, 92, 815-823.                      | 6.5 | 5         |
| 6  | Calibration Methodologies. , 2020, , 213-247.  |     | 2         |
| 7  | Self-Optimized One-Class Classification Using Sum of Ranking Differences Combined with a Receiver Operator Characteristic Curve. <i>Analytical Chemistry</i> , 2020, 92, 5354-5361.            | 6.5 | 10        |
| 8  | Model selection challenges with application to multivariate calibration updating methods. <i>Journal of Chemometrics</i> , 2020, 34, e3245.  | 1.3 | 7         |
| 9  | Application of a Hybrid Fusion Classification Process for Identification of Microplastics Based on Fourier Transform Infrared Spectroscopy. <i>Applied Spectroscopy</i> , 2020, 74, 1167-1183. | 2.2 | 31        |
| 10 | Data Fusion of Nonoptimized Models. <i>Data Handling in Science and Technology</i> , 2019, , 345-370.  | 3.1 | 3         |
| 11 | Sample and feature augmentation strategies for calibration updating. <i>Journal of Chemometrics</i> , 2019, 33, e3080.   | 1.3 | 13        |
| 12 | Feasibility Assessment of Synchronous Fluorescence Spectral Fusion by Application to Argan Oil for Adulteration Analysis. <i>Applied Spectroscopy</i> , 2018, 72, 432-441.                     | 2.2 | 17        |
| 13 | Consensus Classification Using Non-Optimized Classifiers. <i>Analytical Chemistry</i> , 2018, 90, 4429-4437.   | 6.5 | 20        |
| 14 | Sample-wise spectral multivariate calibration desensitized to new artifacts relative to the calibration data using a residual penalty. <i>Journal of Chemometrics</i> , 2017, 31, e2873.       | 1.3 | 7         |
| 15 | Introduction to special issue on penalty methods. <i>Journal of Chemometrics</i> , 2017, 31, e2879.  | 1.3 | 0         |
| 16 | Consensus Outlier Detection Using Sum of Ranking Differences of Common and New Outlier Measures Without Tuning Parameter Selections. <i>Analytical Chemistry</i> , 2017, 89, 5087-5094.        | 6.5 | 32        |
| 17 | Leveraging multiple linear regression for wavelength selection. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017, 168, 121-127.   | 3.5 | 9         |
| 18 | Selectivity-relaxed classical and inverse least squares calibration and selectivity measures with a unified selectivity coefficient. <i>Journal of Chemometrics</i> , 2017, 31, e2925.         | 1.3 | 7         |

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|----|--|-----|-----------|
| 19 | Penalty processes for combining roughness and smoothness in spectral multivariate calibration. <i>Journal of Chemometrics</i> , 2016, 30, 144-152.   | 1.3 | 3         |
| 20 | Using the L 1 norm to select basis set vectors for multivariate calibration and calibration updating. <i>Journal of Chemometrics</i> , 2016, 30, 109-120.  | 1.3 | 3         |
| 21 | Fusion strategies for selecting multiple tuning parameters for multivariate calibration and other penalty based processes: A model updating application for pharmaceutical analysis. <i>Analytica Chimica Acta</i> , 2016, 921, 28-37.               | 5.4 | 27        |
| 22 | Feasibility Study for Transforming Spectral and Instrumental Artifacts for Multivariate Calibration Maintenance. <i>Applied Spectroscopy</i> , 2015, 69, 407-416.  | 2.2 | 10        |
| 23 | Sum of ranking differences (SRD) to ensemble multivariate calibration model merits for tuning parameter selection and comparing calibration methods. <i>Analytica Chimica Acta</i> , 2015, 869, 21-33.   | 5.4 | 39        |
| 24 | Net Analyte Signal (NAS) for Selection of Multivariate Calibration Models and Development of NAS Sample-Wise Target Calibration Model Attributes. <i>ACS Symposium Series</i> , 2015, , 221-240.   | 0.5 | 0         |
| 25 | Characterizing multivariate calibration tradeoffs (bias, variance, selectivity, and sensitivity) to select model tuning parameters. <i>Journal of Chemometrics</i> , 2014, 28, 347-357.  | 1.3 | 32        |
| 26 | Data fusion for food authentication. Combining rare earth elements and trace metals to discriminate "Fava Santorinis" from other yellow split peas using chemometric tools. <i>Food Chemistry</i> , 2014, 165, 316-322.                              | 8.2 | 56        |
| 27 | Food adulteration analysis without laboratory prepared or determined reference food adulterant values. <i>Food Chemistry</i> , 2014, 148, 289-293.   | 8.2 | 10        |
| 28 | Spectral Multivariate Calibration without Laboratory Prepared or Determined Reference Analyte Values. <i>Analytical Chemistry</i> , 2013, 85, 1509-1516.   | 6.5 | 12        |
| 29 | A consensus modeling approach to update a spectroscopic calibration. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2013, 120, 142-153.  | 3.5 | 39        |
| 30 | Interrelationships between generalized Tikhonov regularization, generalized net analyte signal, and generalized least squares for desensitizing a multivariate calibration to interferences. <i>Journal of Chemometrics</i> , 2013, 27, 126-140.     | 1.3 | 15        |
| 31 | 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 adulterant identification. <i>Journal of Chemometrics</i> , 2012, 26, 66-75. | 1.3 | 5         |
| 32 | Overview of two-norm ( $L_{2}$ ) and one-norm ( $L_{1}$ ) Tikhonov regularization variants for full wavelength or sparse spectral multivariate calibration models or maintenance. <i>Journal of Chemometrics</i> , 2012, 26, 218-230.                | 1.3 | 65        |
| 33 | Updating a near-infrared multivariate calibration model formed with lab-prepared pharmaceutical tablet types to new tablet types in full production. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2012, 61, 114-121.                   | 2.8 | 26        |
| 34 | Updating a Synchronous Fluorescence Spectroscopic Virgin Olive Oil Adulteration Calibration to a New Geographical Region. <i>Journal of Agricultural and Food Chemistry</i> , 2011, 59, 1051-1057.   | 5.2 | 38        |
| 35 | Multivariate calibration leverages and spectral $F_{i}$ ratios via the filter factor representation. <i>Journal of Chemometrics</i> , 2010, 24, 249-260.   | 1.3 | 6         |
| 36 | Impact of standardization sample design on Tikhonov regularization variants for spectroscopic calibration maintenance and transfer. <i>Journal of Chemometrics</i> , 2010, 24, 218-229.  | 1.3 | 33        |

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|----|--|------|-----------|
| 37 | Spectral Multivariate Calibration with Wavelength Selection Using Variants of Tikhonov Regularization. <i>Applied Spectroscopy</i> , 2010, 64, 1388-1395.  | 2.2  | 36        |
| 38 | Model Updating for Spectral Calibration Maintenance and Transfer Using 1-Norm Variants of Tikhonov Regularization. <i>Analytical Chemistry</i> , 2010, 82, 3642-3649.                                  | 6.5  | 56        |
| 39 | Calibration Maintenance and Transfer Using Tikhonov Regularization Approaches. <i>Applied Spectroscopy</i> , 2009, 63, 800-809.  | 2.2  | 61        |
| 40 | Learning from Procrustes analysis to improve multivariate calibration. <i>Journal of Chemometrics</i> , 2008, 22, 227-234.   | 1.3  | 16        |
| 41 | Prediction of retention indices for identification of fatty acid methyl esters. <i>Journal of Chromatography A</i> , 2008, 1198-1199, 188-195.   | 3.7  | 27        |
| 42 | A Service-Learning Project Based on a Research Supportive Curriculum Format in the General Chemistry Laboratory. <i>Journal of Chemical Education</i> , 2008, 85, 1410.                                | 2.3  | 41        |
| 43 | Progression of Chemometrics in Research Supportive Curricula: Preparing for the Demands of Society. <i>ACS Symposium Series</i> , 2007, , 140-156.   | 0.5  | 2         |
| 44 | Wavelength Selection for Multivariate Calibration Using Tikhonov Regularization. <i>Applied Spectroscopy</i> , 2007, 61, 85-95.  | 2.2  | 40        |
| 45 | Evaluation of Multivariate Calibration Using a Tikhonov Regularization Approach and the Generalized Pairwise Correlation Method with Nonlinear Data. <i>Analytical Letters</i> , 2007, 40, 1227-1251.  | 1.8  | 1         |
| 46 | Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report). <i>Pure and Applied Chemistry</i> , 2006, 78, 633-661.  | 1.9  | 309       |
| 47 | Impartial graphical comparison of multivariate calibration methods and the harmony/parsimony tradeoff. <i>Journal of Chemometrics</i> , 2006, 20, 464-475.   | 1.3  | 23        |
| 48 | Tikhonov regularization in standardized and general form for multivariate calibration with application towards removing unwanted spectral artifacts. <i>Journal of Chemometrics</i> , 2006, 20, 22-33. | 1.3  | 26        |
| 49 | Multivariate Calibration, an Overview. <i>Analytical Letters</i> , 2005, 38, 2259-2279.  | 1.8  | 46        |
| 50 | Realizing Workplace Skills in Instrumental Analysis. <i>Journal of Chemical Education</i> , 2005, 82, 895.   | 2.3  | 16        |
| 51 | QSAR modeling based on the bias/variance compromise: a harmonious. <i>Journal of Computer-Aided Molecular Design</i> , 2004, 18, 537-547.  | 2.9  | 9         |
| 52 | Effective rank for multivariate calibration methods. <i>Journal of Chemometrics</i> , 2004, 18, 306-311.   | 1.3  | 27        |
| 53 | Pareto calibration with built-in wavelength selection. <i>Analytica Chimica Acta</i> , 2004, 505, 9-14.  | 5.4  | 18        |
| 54 | Quantifying selectivity in spectrophotometric multicomponent analysis. <i>TrAC - Trends in Analytical Chemistry</i> , 2003, 22, 352-361.   | 11.4 | 32        |

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|----|--|-----|-----------|
| 55 | Assessment of Pareto Calibration, Stability, and Wavelength Selection. <i>Applied Spectroscopy</i> , 2003, 57, 309-316.  | 2.2 | 10        |
| 56 | Demonstrated Potential of Ion Mobility Spectrometry for Detection of Adulterated Perfumes and Plant Speciation. <i>Analytical Letters</i> , 2003, 36, 215-244.   | 1.8 | 9         |
| 57 | Graphical diagnostics for regression model determinations with consideration of the bias/variance trade-off. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2002, 60, 173-188.                                     | 3.5 | 45        |
| 58 | Pareto Optimal Multivariate Calibration for Spectroscopic Data. <i>Applied Spectroscopy</i> , 2001, 55, 1645-1652.   | 2.2 | 27        |
| 59 | PCR eigenvector selection based on correlation relative standard deviations. <i>Journal of Chemometrics</i> , 2001, 15, 615-626.   | 1.3 | 12        |
| 60 | Basis sets for multivariate regression. <i>Analytica Chimica Acta</i> , 2001, 428, 31-40.  | 5.4 | 48        |
| 61 | Implementation of Traditional and Real-World Cooperative Learning Techniques in Quantitative Analysis Including Near Infrared Spectroscopy for Analysis of Live Fish. <i>Journal of Chemical Education</i> , 2000, 77, 1314. | 2.3 | 12        |
| 62 | Cyclic subspace regression with analysis of the hat matrix. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1999, 45, 215-224.  | 3.5 | 23        |
| 63 | Interrelationships of multivariate regression methods using eigenvector basis sets. <i>Journal of Chemometrics</i> , 1999, 13, 111-132.  | 1.3 | 68        |
| 64 | Post-Consumer Plastic Identification Using Raman Spectroscopy. <i>Applied Spectroscopy</i> , 1999, 53, 672-681.  | 2.2 | 89        |
| 65 | Fundamentals of Calibration Transfer through Procrustes Analysis. <i>Applied Spectroscopy</i> , 1999, 53, 1268-1276.   | 2.2 | 48        |
| 66 | Cyclic Subspace Regression. <i>Journal of Multivariate Analysis</i> , 1998, 65, 58-70.   | 1.0 | 24        |
| 67 | Orthogonality considerations for library searching Nth-order data. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1998, 41, 115-125.   | 3.5 | 4         |
| 68 | Stabilization of cyclic subspace regression. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1998, 41, 127-134.   | 3.5 | 6         |
| 69 | Use of Matrix Orthogonal Projection for Peak Purity Assessment. <i>Analytical Letters</i> , 1997, 30, 395-416.   | 1.8 | 5         |
| 70 | Wavelength Selection Characterization for NIR Spectra. <i>Applied Spectroscopy</i> , 1997, 51, 689-699.  | 2.2 | 66        |
| 71 | Two data sets of near infrared spectra. <i>Chemometrics and Intelligent Laboratory Systems</i> , 1997, 37, 255-259.  | 3.5 | 191       |
| 72 | Local prediction models by principal component regression. <i>Analytica Chimica Acta</i> , 1997, 348, 29-38.   | 5.4 | 26        |

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|----|---|-----|-----------|
| 73 | Selectivity and Related Measures fourth-Order Data. Analytical Chemistry, 1996, 68, 1572-1579.  | 6.5 | 84        |
| 74 | Simulated-annealing-based optimization algorithms: Fundamentals and wavelength selection applications. Journal of Chemometrics, 1995, 9, 283-308.                               | 1.3 | 42        |
| 75 | A global perspective on multivariate calibration methods. Journal of Chemometrics, 1993, 7, 153-163.  | 1.3 | 7         |
| 76 | Computer-generated multicomponent calibration designs for optimal analysis sample predictions. Journal of Chemometrics, 1992, 6, 85-96.   | 1.3 | 5         |
| 77 | Which principal components to utilize for principal component regression. Journal of Chemometrics, 1992, 6, 217-225.  | 1.3 | 93        |
| 78 | Generalized simulated annealing for calibration sample selection from an existing set and orthogonalization of undesigned experiments. Journal of Chemometrics, 1991, 5, 37-48. | 1.3 | 44        |
| 79 | Assessing Spectral Orthogonality. Applied Spectroscopy Reviews, 1989, 25, 229-259.  | 6.7 | 6         |
| 80 | Variance-decomposition of pure-component spectra as a measure of selectivity. Journal of Chemometrics, 1989, 3, 409-418.  | 1.3 | 17        |
| 81 | Condition numbers, iterative refinement and error bounds. Journal of Chemometrics, 1989, 3, 443-449.  | 1.3 | 6         |
| 82 | Global optimization by simulated annealing with wavelength selection for ultraviolet-visible spectrophotometry. Analytical Chemistry, 1989, 61, 2024-2030.                      | 6.5 | 207       |
| 83 | A Simplex Optimized Inductively Coupled Plasma Spectrometer with Minimization of Interferences. Applied Spectroscopy, 1987, 41, 1338-1342.                                      | 2.2 | 12        |
| 84 | Restoration of defaced serial numbers using lock-in infrared thermography (Part I). Journal of Spectral Imaging, 0, , .   | 0.0 | 2         |
| 85 | Restoration of defaced serial numbers using lock-in infrared thermography (Part II). Journal of Spectral Imaging, 0, , .  | 0.0 | 1         |