John H Kalivas

List of Publications by Year
in descending order

85	2,647	186265	197818
papers	citations	28 h-index	49 g-index

89	89	89	1814
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Uncertainty estimation and figures of merit for multivariate calibration (IUPAC Technical Report). Pure and Applied Chemistry, 2006, 78, 633-661.	1.9	309
2	Global optimization by simulated annealing with wavelength selection for ultraviolet-visible spectrophotometry. Analytical Chemistry, 1989, 61, 2024-2030.	6.5	207
3	Two data sets of near infrared spectra. Chemometrics and Intelligent Laboratory Systems, 1997, 37, 255-259.	3.5	191
4	Which principal components to utilize for principal component regression. Journal of Chemometrics, 1992, 6, 217-225.	1.3	93
5	Post-Consumer Plastic Identification Using Raman Spectroscopy. Applied Spectroscopy, 1999, 53, 672-681.	2.2	89
6	Selectivity and Related Measures fornth-Order Data. Analytical Chemistry, 1996, 68, 1572-1579.	6.5	84
7	Interrelationships of multivariate regression methods using eigenvector basis sets. Journal of Chemometrics, 1999, 13, 111-132.	1.3	68
8	Wavelength Selection Characterization for NIR Spectra. Applied Spectroscopy, 1997, 51, 689-699.	2.2	66
9	Overview of twoâ€•norm (L₂) and oneâ€•norm (L₁) Tikhonov regularization variants for full wavelength or sparse spectral multivariate calibration models or maintenance. Journal of Chemometrics, 2012, 26, 218-230.	1.3	65
10	Calibration Maintenance and Transfer Using Tikhonov Regularization Approaches. Applied Spectroscopy, 2009, 63, 800-809.	2.2	61
11	Model Updating for Spectral Calibration Maintenance and Transfer Using 1-Norm Variants of Tikhonov Regularization. Analytical Chemistry, 2010, 82, 3642-3649.	6.5	56
12	Data fusion for food authentication. Combining rare earth elements and trace metals to discriminate â€œFava Santorinisâ€•from other yellow split peas using chemometric tools. Food Chemistry, 2014, 165, 316-322.	8.2	56
13	Fundamentals of Calibration Transfer through Procrustes Analysis. Applied Spectroscopy, 1999, 53, 1268-1276.	2.2	48
14	Basis sets for multivariate regression. Analytica Chimica Acta, 2001, 428, 31-40.	5.4	48
15	Multivariate Calibration, an Overview. Analytical Letters, 2005, 38, 2259-2279.	1.8	46
16	Graphical diagnostics for regression model determinations with consideration of the bias/variance trade-off. Chemometrics and Intelligent Laboratory Systems, 2002, 60, 173-188.	3.5	45
17	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
18	Simulated-annealing-based optimization algorithms: Fundamentals and wavelength selection applications. Journal of Chemometrics, 1995, 9, 283-308.	1.3	42

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19	A Service-Learning Project Based on a Research Supportive Curriculum Format in the General Chemistry Laboratory. Journal of Chemical Education, 2008, 85, 1410.	2.3	41
20	Wavelength Selection for Multivariate Calibration Using Tikhonov Regularization. Applied Spectroscopy, 2007, 61, 85-95.	2.2	40
21	A consensus modeling approach to update a spectroscopic calibration. Chemometrics and Intelligent Laboratory Systems, 2013, 120, 142-153.	3.5	39
22	Sum of ranking differences (SRD) to ensemble multivariate calibration model merits for tuning parameter selection and comparing calibration methods. Analytica Chimica Acta, 2015, 869, 21-33.	5.4	39
23	Updating a Synchronous Fluorescence Spectroscopic Virgin Olive Oil Adulteration Calibration to a New Geographical Region. Journal of Agricultural and Food Chemistry, 2011, 59, 1051-1057.	5.2	38
24	Spectral Multivariate Calibration with Wavelength Selection Using Variants of Tikhonov Regularization. Applied Spectroscopy, 2010, 64, 1388-1395.	2.2	36
25	Impact of standardization sample design on Tikhonov regularization variants for spectroscopic calibration maintenance and transfer. Journal of Chemometrics, 2010, 24, 218-229.	1.3	33
26	Quantifying selectivity in spectrophotometric multicomponent analysis. TrAC - Trends in Analytical Chemistry, 2003, 22, 352-361.	11.4	32
27	Characterizing multivariate calibration tradeoffs (bias, variance, selectivity, and sensitivity) to select model tuning parameters. Journal of Chemometrics, 2014, 28, 347-357.	1.3	32
28	Consensus Outlier Detection Using Sum of Ranking Differences of Common and New Outlier Measures Without Tuning Parameter Selections. Analytical Chemistry, 2017, 89, 5087-5094.	6.5	32
29	Application of a Hybrid Fusion Classification Process for Identification of Microplastics Based on Fourier Transform Infrared Spectroscopy. Applied Spectroscopy, 2020, 74, 1167-1183.	2.2	31
30	Pareto Optimal Multivariate Calibration for Spectroscopic Data. Applied Spectroscopy, 2001, 55, 1645-1652.	2.2	27
31	Effective rank for multivariate calibration methods. Journal of Chemometrics, 2004, 18, 306-311.	1.3	27
32	Prediction of retention indices for identification of fatty acid methyl esters. Journal of Chromatography A, 2008, 1198-1199, 188-195.	3.7	27
33	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, 2016, 921, 28-37.	5.4	27
34	Local prediction models by principal component regression. Analytica Chimica Acta, 1997, 348, 29-38.	5.4	26
35	Tikhonov regularization in standardized and general form for multivariate calibration with application towards removing unwanted spectral artifacts. Journal of Chemometrics, 2006, 20, 22-33.	1.3	26
36	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, 2012, 61, 114-121.	2.8	26

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37	Cyclic Subspace Regression. Journal of Multivariate Analysis, 1998, 65, 58-70.	1.0	24
38	Cyclic subspace regression with analysis of the hat matrix. Chemometrics and Intelligent Laboratory Systems, 1999, 45, 215-224.	3.5	23
39	Impartial graphical comparison of multivariate calibration methods and the harmony/parsimony tradeoff. Journal of Chemometrics, 2006, 20, 464-475.	1.3	23
40	Consensus Classification Using Non-Optimized Classifiers. Analytical Chemistry, 2018, 90, 4429-4437.	6.5	20
41	Pareto calibration with built-in wavelength selection. Analytica Chimica Acta, 2004, 505, 9-14.	5.4	18
42	Variance-decomposition of pure-component spectra as a measure of selectivity. Journal of Chemometrics, 1989, 3, 409-418.	1.3	17
43	Feasibility Assessment of Synchronous Fluorescence Spectral Fusion by Application to Argan Oil for Adulteration Analysis. Applied Spectroscopy, 2018, 72, 432-441.	2.2	17
44	Realizing Workplace Skills in Instrumental Analysis. Journal of Chemical Education, 2005, 82, 895.	2.3	16
45	Learning from Procrustes analysis to improve multivariate calibration. Journal of Chemometrics, 2008, 22, 227-234.	1.3	16
46	Interrelationships between generalized Tikhonov regularization, generalized net analyte signal, and generalized least squares for desensitizing a multivariate calibration to interferences. Journal of Chemometrics, 2013, 27, 126-140.	1.3	15
47	Sample and feature augmentation strategies for calibration updating. Journal of Chemometrics, 2019, 33, e3080.	1.3	13
48	A Simplex Optimized Inductively Coupled Plasma Spectrometer with Minimization of Interferences. Applied Spectroscopy, 1987, 41, 1338-1342.	2.2	12
49	Implementation of Traditional and Real-World Cooperative Learning Techniques in Quantitative Analysis Including Near Infrared Spectroscopy for Analysis of Live Fish. Journal of Chemical Education, 2000, 77, 1314.	2.3	12
50	PCR eigenvector selection based on correlation relative standard deviations. Journal of Chemometrics, 2001, 15, 615-626.	1.3	12
51	Spectral Multivariate Calibration without Laboratory Prepared or Determined Reference Analyte Values. Analytical Chemistry, 2013, 85, 1509-1516.	6.5	12
52	Ultrasonic-assisted catalytic transfer hydrogenation for upgrading pyrolysis-oil. Ultrasonics Sonochemistry, 2021, 73, 105502.	8.2	11
53	Assessment of Pareto Calibration, Stability, and Wavelength Selection. Applied Spectroscopy, 2003, 57, 309-316.	2.2	10
54	Food adulteration analysis without laboratory prepared or determined reference food adulterant values. Food Chemistry, 2014, 148, 289-293.	8.2	10

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55	Feasibility Study for Transforming Spectral and Instrumental Artifacts for Multivariate Calibration Maintenance. Applied Spectroscopy, 2015, 69, 407-416.	2.2	10
56	Self-Optimized One-Class Classification Using Sum of Ranking Differences Combined with a Receiver Operator Characteristic Curve. Analytical Chemistry, 2020, 92, 5354-5361.	6.5	10
57	Demonstrated Potential of Ion Mobility Spectrometry for Detection of Adulterated Perfumes and Plant Speciation. Analytical Letters, 2003, 36, 215-244.	1.8	9
58	QSAR modeling based on the bias/variance compromise: a harmonious. Journal of Computer-Aided Molecular Design, 2004, 18, 537-547.	2.9	9
59	Leveraging multiple linear regression for wavelength selection. Chemometrics and Intelligent Laboratory Systems, 2017, 168, 121-127.	3.5	9
60	A global perspective on multivariate calibration methods. Journal of Chemometrics, 1993, 7, 153-163.	1.3	7
61	Sampleâ€wise spectral multivariate calibration desensitized to new artifacts relative to the calibration data using a residual penalty. Journal of Chemometrics, 2017, 31, e2873.	1.3	7
62	Selectivityâ€relaxed classical and inverse least squares calibration and selectivity measures with a unified selectivity coefficient. Journal of Chemometrics, 2017, 31, e2925.	1.3	7
63	Model selection challenges with application to multivariate calibration updating methods. Journal of Chemometrics, 2020, 34, e3245.	1.3	7
64	Calibration Model Updating to Novel Sample and Measurement Conditions without Reference Values. Analytical Chemistry, 2021, 93, 9688-9696.	6.5	7
65	Assessing Spectral Orthogonality. Applied Spectroscopy Reviews, 1989, 25, 229-259.	6.7	6
66	Condition numbers, iterative refinement and error bounds. Journal of Chemometrics, 1989, 3, 443-449.	1.3	6
67	Stabilization of cyclic subspace regression. Chemometrics and Intelligent Laboratory Systems, 1998, 41, 127-134.	3.5	6
68	Multivariate calibration leverages and spectral Fâ€ratios via the filter factor representation. Journal of Chemometrics, 2010, 24, 249-260.	1.3	6
69	Computer-generated multicomponent calibration designs for optimal analysis sample predictions. Journal of Chemometrics, 1992, 6, 85-96.	1.3	5
70	Use of Matrix Orthogonal Projection for Peak Purity Assessment. Analytical Letters, 1997, 30, 395-416.	1.8	5
71	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. Journal of Chemometrics, 2012, 26, 66-75.	1.3	5
72	Identifying Chemical, Physical, and Instrumental Matrix Matched Samples by Leveraging Spectral Model Regression Vectors. Analytical Chemistry, 2020, 92, 815-823.	6.5	5

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73	Reliable Model Selection without Reference Values by Utilizing Model Diversity with Prediction Similarity. Journal of Chemical Information and Modeling, 2021, 61, 2220-2230.	5.4	5
74	Orthogonality considerations for library searching Nth-order data. Chemometrics and Intelligent Laboratory Systems, 1998, 41, 115-125.	3.5	4
75	Penalty processes for combining roughness and smoothness in spectral multivariate calibration. Journal of Chemometrics, 2016, 30, 144-152.	1.3	3
76	Using the L 1 norm to select basis set vectors for multivariate calibration and calibration updating. Journal of Chemometrics, 2016, 30, 109-120.	1.3	3
77	Data Fusion of Nonoptimized Models. Data Handling in Science and Technology, 2019, , 345-370.	3.1	3
78	Progression of Chemometrics in Research Supportive Curricula: Preparing for the Demands of Society. ACS Symposium Series, 2007, , 140-156.	0.5	2
79	Calibration Methodologies. , 2020, , 213-247.		2
80	Automatic food and beverage authentication and adulteration detection by classification hybrid fusion. Journal of Chemometrics, 2023, 37, e3371.	1.3	2
81	Restoration of defaced serial numbers using lock-in infrared thermography (Part I). Journal of Spectral Imaging, 0, , .	0.0	2
82	Evaluation of Multivariate Calibration Using a Tikhonov Regularization Approach and the Generalized Pairâ€Correlation Method with Nonlinear Data. Analytical Letters, 2007, 40, 1227-1251.	1.8	1
83	Restoration of defaced serial numbers using lock-in infrared thermography (Part II). Journal of Spectral Imaging, 0, , .	0.0	1
84	Net Analyte Signal (NAS) for Selection of Multivariate Calibration Models and Development of NAS Sample-Wise Target Calibration Model Attributes. ACS Symposium Series, 2015, , 221-240.	0.5	0
85	Introduction to special issue on penalty methods. Journal of Chemometrics, 2017, 31, e2879.	1.3	0