Gary W Small

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Genetic Algorithm-Based Method for Selecting Wavelengths and Model Size for Use with Partial Least-Squares Regression:Â Application to Near-Infrared Spectroscopy. Analytical Chemistry, 1996, 68, 4200-4212.	6.5	186
2	Determination of physiological levels of glucose in an aqueous matrix with digitally filtered Fourier transform near-infrared spectra. Analytical Chemistry, 1990, 62, 1457-1464.	6.5	155
3	Noninvasive Glucose Sensing. Analytical Chemistry, 2005, 77, 5429-5439.	6.5	144
4	Temperature-Insensitive Near-Infrared Spectroscopic Measurement of Glucose in Aqueous Solutions. Applied Spectroscopy, 1994, 48, 477-483.	2.2	122
5	Measurement of glucose and other analytes in undiluted human serum with near-infrared transmission spectroscopy. Analytica Chimica Acta, 1998, 371, 255-267.	5.4	115
6	Phantom Glucose Calibration Models from Simulated Noninvasive Human Near-Infrared Spectra. Analytical Chemistry, 1998, 70, 1773-1781.	6.5	115
7	Comparison of Combination and First Overtone Spectral Regions for Near-Infrared Calibration Models for Glucose and Other Biomolecules in Aqueous Solutions. Analytical Chemistry, 2004, 76, 5405-5413.	6.5	112
8	Strategies for coupling digital filtering with partial least-squares regression: Application to the determination of glucose in plasma by Fourier-transform near-infrared spectroscopy. Analytical Chemistry, 1993, 65, 3279-3289.	6.5	109
9	Near-Infrared Spectroscopic Measurement of Physiological Glucose Levels in Variable Matrices of Protein and Triglycerides. Analytical Chemistry, 1996, 68, 1124-1135.	6.5	97
10	Measurement of Glucose in Water with First-Overtone Near-Infrared Spectra. Applied Spectroscopy, 1998, 52, 1597-1605.	2.2	90
11	Noninvasive Blood Glucose Measurements by Near-Infrared Transmission Spectroscopy Across Human Tongues. Diabetes Technology and Therapeutics, 2000, 2, 5-16.	4.4	85
12	Genetic Algorithm-Based Wavelength Selection for the Near-Infrared Determination of Glucose in Biological Matrixes:Â Initialization Strategies and Effects of Spectral Resolution. Analytical Chemistry, 1998, 70, 4472-4479.	6.5	80
13	Near-infrared spectroscopic measurement of glucose in a protein matrix. Analytical Chemistry, 1993, 65, 3271-3278.	6.5	78
14	Scattering and Absorption Effects in the Determination of Glucose in Whole Blood by Near-Infrared Spectroscopy. Analytical Chemistry, 2005, 77, 4587-4594.	6.5	73
15	Chemometrics and near-infrared spectroscopy: Avoiding the pitfalls. TrAC - Trends in Analytical Chemistry, 2006, 25, 1057-1066.	11.4	73
16	Genetic Algorithm-Based Protocol for Coupling Digital Filtering and Partial Least-Squares Regression:Â Application to the Near-Infrared Analysis of Glucose in Biological Matrices. Analytical Chemistry, 1996, 68, 2663-2675.	6.5	64
17	Detection of atmospheric pollutants by direct analysis of passive Fourier transform infrared interferograms. Analytical Chemistry, 1988, 60, 264-269.	6.5	61
18	Design of optimized finite impulse response digital filters for use with passive Fourier transform infrared interferograms. Analytical Chemistry, 1990, 62, 1768-1777.	6.5	57

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19	Classification of Fourier Transform Infrared Microscopic Imaging Data of Human Breast Cells by Cluster Analysis and Artificial Neural Networks. Applied Spectroscopy, 2003, 57, 14-22.	2.2	53
20	Peer Reviewed: Learning Optimization From Nature: Genetic Algorithms and Simulated Annealing. Analytical Chemistry, 1997, 69, 236A-242A.	6.5	50
21	Interactive computer system for the simulation of carbon-13 nuclear magnetic resonance spectra. Analytical Chemistry, 1983, 55, 1121-1127.	6.5	48
22	Multivariate Calibration Standardization across Instruments for the Determination of Glucose by Fourier Transform Near-Infrared Spectrometry. Analytical Chemistry, 2003, 75, 5905-5915.	6.5	45
23	Development and optimization of piecewise linear discriminants for the automated detection of chemical species. Analytical Chemistry, 1991, 63, 936-944.	6.5	44
24	Pure Component Selectivity Analysis of Multivariate Calibration Models from Near-Infrared Spectra. Analytical Chemistry, 2004, 76, 2583-2590.	6.5	44
25	Automated detection of methanol vapour by open path Fourier transform infrared spectrometry. Analytica Chimica Acta, 1994, 297, 387-403.	5.4	41
26	Spectral Simulation Methodology for Calibration Transfer of Near-Infrared Spectra. Applied Spectroscopy, 2007, 61, 406-413.	2.2	40
27	Automated Detection of Trichloroethylene by Fourier Transform Infrared Remote Sensing Measurements. Analytical Chemistry, 1997, 69, 118-129.	6.5	39
28	Determination of Glucose in a Biological Matrix by Multivariate Analysis of Multiple Band-Pass-Filtered Fourier Transform Near-Infrared Interferograms. Analytical Chemistry, 1997, 69, 4695-4702.	6.5	38
29	Calibration Standardization Algorithm for Partial Least-Squares Regression:Â Application to the Determination of Physiological Levels of Glucose by Near-Infrared Spectroscopy. Analytical Chemistry, 2002, 74, 4097-4108.	6.5	38
30	Simulation of carbon-13 nuclear magnetic resonance spectra of cycloalkanols with computer-based structural descriptors. Analytical Chemistry, 1983, 55, 1128-1134.	6.5	36
31	Determination of topological similarity of carbon atoms in the simulation of carbon-13 nuclear magnetic resonance spectra. Analytical Chemistry, 1984, 56, 1314-1323.	6.5	35
32	Selection of optimum training sets for use in pattern recognition analysis of chemical data. Analytica Chimica Acta, 1991, 249, 305-321.	5.4	35
33	Rapid signal processing techniques for Fourier transform infrared remote sensing. TrAC - Trends in Analytical Chemistry, 1991, 10, 149-155.	11.4	32
34	Data reduction in the simulation of carbon-13 nuclear magnetic resonance spectra of steroids. Analytical Chemistry, 1984, 56, 2307-2314.	6.5	31
35	Improved response function for the Simplex optimization of piecewise linear discriminants. Chemometrics and Intelligent Laboratory Systems, 1996, 32, 95-109.	3.5	30
36	Carbon-13 nuclear magnetic resonance spectrum simulation methodology for the structure elucidation of carbohydrates. Analytical Chemistry, 1987, 59, 1805-1811.	6.5	29

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37	Calibration Transfer Algorithm for Automated Qualitative Analysis by Passive Fourier Transform Infrared Spectrometry. Analytical Chemistry, 2000, 72, 1690-1698.	6.5	27
38	Remote Detection of Volatile Organic Compounds by Passive Multispectral Infrared Imaging Measurements. Applied Spectroscopy, 2007, 61, 349-358.	2.2	24
39	Advanced nearâ€infrared monitor for stable realâ€time measurement and control of <i>Pichia pastoris</i> bioprocesses. Biotechnology Progress, 2014, 30, 749-759.	2.6	24
40	Evaluation of selectivity and robustness of near-infrared glucose measurements based on short-scan Fourier transform infrared interferograms. Analytica Chimica Acta, 2003, 490, 325-340.	5.4	23
41	Quantitative Analysis of Bandpass-Filtered Fourier Transform Infrared Interferograms. Analytical Chemistry, 1995, 67, 2269-2278.	6.5	22
42	Real-time monitoring of glycerol and methanol to enhance antibody production in industrial Pichia pastoris bioprocesses. Biochemical Engineering Journal, 2015, 94, 115-124.	3.6	22
43	Evaluation of nonlinear model building strategies for the determination of glucose in biological matrices by near-infrared spectroscopy. Analytica Chimica Acta, 1999, 384, 333-343.	5.4	21
44	Evaluation of Data Pretreatment and Model Building Methods for the Determination of Glucose from Near-Infrared Single-Beam Spectra. Applied Spectroscopy, 1999, 53, 402-414.	2.2	21
45	Automated Detection of Chemical Vapors by Pattern Recognition Analysis of Passive Multispectral Infrared Remote Sensing Imaging Data. Applied Spectroscopy, 2002, 56, 1082-1093.	2.2	21
46	Quantitative Analysis of Sulfur Dioxide with Passive Fourier Transform Infrared Remote Sensing Interferogram Data. Applied Spectroscopy, 2000, 54, 341-348.	2.2	20
47	Simulation of carbon-13 nuclear magnetic resonance spectra of polycyclic aromatic compounds. Analytical Chemistry, 1991, 63, 1081-1090.	6.5	19
48	Multivariate Calibration Models Based on the Direct Analysis of Near-Infrared Single-Beam Spectra. Applied Spectroscopy, 1997, 51, 1330-1339.	2.2	19
49	Wavelet analysis used for spectral background removal in the determination of glucose from near-infrared single-beam spectra. Analytica Chimica Acta, 2010, 681, 63-70.	5.4	19
50	Automated spectral interpretation. Analytical Chemistry, 1987, 59, 535A-546A.	6.5	18
51	Automated selection of library subsets for infrared spectral searching. Analytical Chemistry, 1990, 62, 226-233.	6.5	18
52	Remote Detection of Heated Ethanol Plumes by Airborne Passive Fourier Transform Infrared Spectrometry. Applied Spectroscopy, 2003, 57, 1432-1441.	2.2	18
53	Automated detection of sulfur dioxide in stack emissions by passive Fourier transform infrared spectrometry. Vibrational Spectroscopy, 2001, 27, 97-107.	2.2	17
54	Blank Augmentation Protocol for Improving the Robustness of Multivariate Calibrations. Applied Spectroscopy, 2007, 61, 497-506.	2.2	17

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55	Structure elucidation methodology for disaccharides based on carbon-13 nuclear magnetic resonance spectrum simulation. Analytical Chemistry, 1989, 61, 666-674.	6.5	16
56	Discriminant analysis techniques for the identification of atmospheric pollutants from passive Fourier transform infrared interferograms. Analytica Chimica Acta, 1991, 246, 85-102.	5.4	16
57	Determination of glucose in a synthetic biological matrix with decimated time-domain filtered near-infrared interferogram data. Vibrational Spectroscopy, 2000, 23, 103-117.	2.2	15
58	Digital Filtering and Model Updating Methods for Improving the Robustness of Near-Infrared Multivariate Calibrations. Applied Spectroscopy, 2009, 63, 246-255.	2.2	15
59	Artificial Neural Networks for the Automated Detection of Trichloroethylene by Passive Fourier Transform Infrared Spectrometry. Analytical Chemistry, 2000, 72, 1680-1689.	6.5	14
60	Comparison of optimization algorithms for piecewise linear discriminant analysis: application to Fourier transform infrared remote sensing measurements. Analytica Chimica Acta, 1996, 331, 157-175.	5.4	13
61	Application of Multivariate Calibration Techniques to Quantitative Analysis of Bandpass-Filtered Fourier Transform Infrared Interferogram Data. Applied Spectroscopy, 1997, 51, 1369-1376.	2.2	13
62	Airborne passive Fourier transform infrared remote sensing of methanol vapor from industrial emissions. Analyst, The, 2008, 133, 1776.	3.5	13
63	Determination of moisture content of polyamide 66 directly from combination region nearâ€infrared spectra. Journal of Applied Polymer Science, 2014, 131, .	2.6	13
64	Automated selection of models for the simulation of carbon-13 nuclear magnetic resonance spectra. Analytical Chemistry, 1984, 56, 2314-2319.	6.5	12
65	Robust Classifier for the Automated Detection of Ammonia in Heated Plumes by Passive Fourier Transform Infrared Spectrometry. Analytical Chemistry, 2003, 75, 2018-2026.	6.5	12
66	Determination of Organic Contaminants in Aqueous Samples by Near-Infrared Spectroscopy. Applied Spectroscopy, 2000, 54, 1047-1054.	2.2	11
67	Multiple Filtering Strategy for the Automated Detection of Ethanol by Passive Fourier Transform Infrared Spectrometry. Applied Spectroscopy, 2001, 55, 1544-1552.	2.2	11
68	Reconstruction of gas chromatograms from digitally filtered Fourier-transform infrared interferograms. Analytical Chemistry, 1989, 61, 1073-1079.	6.5	10
69	Automated Spectrum Simulation Methods for Carbon-13 Nuclear Magnetic Resonance Spectroscopy Based on Database Retrieval and Model-Building Strategies. Journal of Chemical Information and Computer Sciences, 1997, 37, 249-257.	2.8	9
70	Calibration Transfer in the Automated Detection of Acetone by Passive Fourier Transform Infrared Spectrometry. Applied Spectroscopy, 2000, 54, 706-714.	2.2	9
71	Robust absorbance computations in the analysis of glucose by near-infrared spectroscopy. Vibrational Spectroscopy, 2007, 43, 440-446.	2.2	9
72	Multivariate Calibration with Basis Functions Derived from Optical Filters. Analytical Chemistry, 2009, 81, 2199-2207.	6.5	9

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73	Quantitative Determination of Methanol and Ethanol with Synthetic Calibration Spectra in Passive Fourier Transform Infrared Remote Sensing Measurements. Applied Spectroscopy, 2013, 67, 913-923.	2.2	9
74	Enhanced Structural Encoding Algorithm for Database Retrievals of Carbon-13 Nuclear Magnetic Resonance Chemical Shifts. Journal of Chemical Information and Computer Sciences, 1996, 36, 310-322.	2.8	8
75	Database retrieval techniques for carbon-13 nuclear magnetic resonance spectrum simulation. Journal of Chemical Information and Computer Sciences, 1992, 32, 279-285.	2.8	7
76	Effect of Spectral Resolution on Pattern Recognition Analysis Using Passive Fourier Transform Infrared Sensor Data. Applied Spectroscopy, 1999, 53, 1382-1391.	2.2	7
77	High-pass filters for spectral background suppression in airborne passive Fourier transform infrared spectrometry. Analytica Chimica Acta, 2004, 501, 235-247.	5.4	7
78	Infinite impulse response filters for direct analysis of interferogram data from airborne passive Fourier transform infrared spectrometry. Vibrational Spectroscopy, 2005, 37, 39-52.	2.2	7
79	Spectral Simulation Protocol for Extending the Lifetime of Near-Infrared Multivariate Calibrations. Analytical Chemistry, 2009, 81, 1208-1216.	6.5	7
80	Design Considerations for Near-Infrared Filter Photometry: Effects of Noise Sources and Selectivity. Applied Spectroscopy, 2009, 63, 700-708.	2.2	7
81	Simulation of carbon-13 nuclear magnetic resonance spectra of linear cyclic aromatic compounds. Analytical Chemistry, 1989, 61, 2658-2664.	6.5	6
82	Quantitative determination of ethanol in heated plumes by passive Fourier transform infrared remote sensing measurements. Analyst, The, 2007, 132, 330.	3.5	6
83	Automated detection of radioisotopes from an aircraft platform by pattern recognition analysis of gamma-ray spectra. Journal of Environmental Radioactivity, 2018, 192, 654-666.	1.7	6
84	Signal Processing Techniques for Remote Infrared Chemical Sensing. , 1990, , 71-111.		6
85	Effects of Data Sampling Rate on Pattern Recognition Analysis of FT-IR Interferograms. Applied Spectroscopy, 1992, 46, 49-59.	2.2	5
86	Simulated Radiance Profiles for Automating the Interpretation of Airborne Passive Multi-Spectral Infrared Images. Applied Spectroscopy, 2008, 62, 1049-1059.	2.2	5
87	Background correction method for improving the automated detection of radioisotopes from airborne gamma-ray surveys. Journal of Environmental Radioactivity, 2019, 198, 104-116.	1.7	5
88	Committee classifier based on linear discriminant analysis for the detection of radioisotopes from airborne gamma-ray spectra. Journal of Environmental Radioactivity, 2020, 217, 106217.	1.7	5
89	Application of visual spectral matching techniques to automated carbon-13 nuclear magnetic resonance library searching. Analytical Chemistry, 1988, 60, 1886-1895.	6.5	4
90	The Effect of Length and Diameter on the Signal-to-Noise Ratio of Evanescent Field Absorption Fiber-Optic Sensors. Applied Spectroscopy, 1992, 46, 1129-1133.	2.2	4

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91	Ridge regression techniques for the optimization of piecewise linear discriminants: application to Fourier transform infrared remote sensing measurements. Analytica Chimica Acta, 1993, 279, 309-322.	5.4	4
92	Performance Enhancement of Vector-Based Search Systems:  Application to Carbon-13 Nuclear Magnetic Resonance Chemical Shift Prediction. Journal of Chemical Information and Computer Sciences, 1996, 36, 46-53.	2.8	4
93	Digital Filtering Implementations for the Detection of Broad Spectral Features by Direct Analysis of Passive Fourier Transform Infrared Interferograms. Applied Spectroscopy, 2004, 58, 432-441.	2.2	4
94	Application of Dynamical Analysis Techniques in the Extraction of Compound-Specific Information from Fourier Transform Infrared Interferograms. Applied Spectroscopy, 1992, 46, 1790-1798.	2.2	3
95	Effects of Bandwidth and Overlap on Multivariate Calibration Models Based on Simulated Fourier Transform Infrared Interferogram Data. Applied Spectroscopy, 1999, 53, 1556-1566.	2.2	3
96	Synthetic training sets for the development of discriminant functions for the detection of volatile organic compounds from passive infrared remote sensing data. Analyst, The, 2011, 136, 309-316.	3.5	3
97	Threshold concentration monitoring based on pattern recognition analysis of differential near-infrared spectra. RSC Advances, 2014, 4, 35405-35414.	3.6	3
98	Determination of temperatures of polyamide 66 directly from nearâ€infrared spectra. Journal of Applied Polymer Science, 2014, 131, .	2.6	3
99	Determination of temperatures of aqueous-based samples directly from near infrared spectra. Journal of Near Infrared Spectroscopy, 2017, 25, 289-300.	1.5	3
100	Nocturnal hypoglycemic alarm based on near-infrared spectroscopy: InÂvitro simulation studies. Analytica Chimica Acta, 2017, 987, 81-90.	5.4	3
101	Neural networks for the automated detection of methanol vapour from airborne passive infrared multispectral imaging data. International Journal of Remote Sensing, 2020, 41, 6698-6717.	2.9	3
102	Longitudinal Study Comparing Orthogonal Signal Correction Algorithms Coupled with Partial Least-Squares for Quantitative Near-Infrared Spectroscopy. Analytical Letters, 2022, 55, 449-466.	1.8	3
103	Real-Time Radionuclide Identification and Mapping Capabilities of the U.S. Environmental Protection Agency's Airborne Spectral Photometric Environmental Collection Technology. NATO Science for Peace and Security Series B: Physics and Biophysics, 2015, , 105-116.	0.3	3
104	Application of parallel processing techniques to improving the efficiency of MM2 molecular mechanics calculations. Journal of Computational Chemistry, 1993, 14, 977-985.	3.3	2
105	Effects of Spectral Resolution on the Determination of Clucose in a Simulated Biological Matrix by Fourier Transform near Infrared Spectrometry. Journal of Near Infrared Spectroscopy, 2006, 14, 291-299.	1.5	2
106	Design and characterization of protein films for modeling near-infrared spectra of human tissue. Analyst, The, 2015, 140, 3981-3988.	3.5	2
107	Determination of structural similarity by quantitative comparisons of Wiswesser Line Notation entries. Journal of Chemical Information and Computer Sciences, 1990, 30, 73-80.	2.8	1
108	Calibration diagnostic and updating strategy based on quantitative modeling of near-infrared spectral residuals. Analyst, The, 2015, 140, 786-796.	3.5	1

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109	Nocturnal Hypoglycemic Alarm Based on Near-Infrared Spectroscopy: In Vivo Studies with a Rat Animal Model. Analytical Chemistry, 2019, 91, 1855-1862.	6.5	1
110	Computer Software Review. Microsoft, Version 4.0. Journal of Chemical Information and Computer Sciences, 1988, 28, 234-235.	2.8	0
111	Computer Software Reviews. NMR simulator and IR simulator. Journal of Chemical Information and Computer Sciences, 1988, 28, 232-234.	2.8	0
112	Books: Fourier Transform for Beginners. Analytical Chemistry, 1996, 68, 738A-738A.	6.5	0
113	Software: Fitting Data to Models. Analytical Chemistry, 1996, 68, 368A-369A.	6.5	0
114	Books: Advanced methods and data processing. Analytical Chemistry, 1997, 69, 424A-424A.	6.5	0
115	Passive Airborne Fourier Transform Infrared Remote Detection of Methanol by Use of Wavelet Analysis as A Feature Extraction Method. Analytical Letters, 2019, 52, 2251-2265.	1.8	0
116	Temperature correction strategy for improving concentration predictions with near-infrared spectra of aqueous-based samples. Analytica Chimica Acta, 2020, 1095, 20-29.	5.4	0