James J Harynuk

List of Publications by Year
in descending order

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81 papers	2,052 citations	218381 26 h-index	264894 42 g-index
84 all docs	84 docs citations	84 times ranked	1567 citing authors

#	Article	IF	Citations
1	Investigation of the accelerated thermal aging behavior of polyetherimide and lifetime prediction at elevated temperature. Journal of Applied Polymer Science, 2022, 139, 51955.	1.3	10
2	Global metabolome analysis of Dunaliella tertiolecta, Phaeobacter italicus R11 Co-cultures using thermal desorption - Comprehensive two-dimensional gas chromatography - Time-of-flight mass spectrometry (TD-GCÃ—GC-TOFMS). Phytochemistry, 2022, 195, 113052.	1.4	8
3	Evaluation of fresh, frozen, and lyophilized fecal samples by SPME and derivatization methods using GCÃ—GC-TOFMS. Metabolomics, 2022, 18, 25.	1.4	3
4	Henryâ€™s Law Constants and Indoor Partitioning of Microbial Volatile Organic Compounds. Environmental Science & Technology, 2022, 56, 7143-7152.	4.6	8
5	Sensitive and Representative Extraction of Petroleum-Based Ignitable Liquids From Fire Debris For Confirmatory Analysis of Canine-Selected Exhibits. Frontiers in Analytical Science, 2022, 2, .	1.1	0
6	Review of Variable Selection Methods for Discriminant-Type Problems in Chemometrics. Frontiers in Analytical Science, 2022, 2, .	1.1	5
7	An efficient and accurate numerical determination of the cluster resolution metric in two dimensions. Journal of Chemometrics, 2021, 35, e3346.	0.7	6
8	Unique ion filterâ€”A data reduction tool for chemometric analysis of raw comprehensive twoâ€dimensional gas chromatographyâ€mass spectrometry data. Journal of Separation Science, 2021, 44, 2773-2784.	1.3	5
9	Automated Screening and Filtering Scripts for GCÃ—GC-TOFMS Metabolomics Data. Separations, 2021, 8, 84.	1.1	11
10	Chemical Characterization of Emissions Arising from Solid Fuel Combustionâ€”Contrasting Wood and Cow Dung Burning. ACS Earth and Space Chemistry, 2021, 5, 2925-2937.	1.2	6
11	Towards Standardization of Data Normalization Strategies to Improve Urinary Metabolomics Studies by GCÃ—GC-TOFMS. Metabolites, 2020, 10, 376.	1.3	28
12	Infection of canola by the root pathogen Plasmodiophora brassicae increases resistance to aboveground herbivory by bertha armyworm, Mamestra configurata Walker (Lepidoptera: Noctuidae). Plant Science, 2020, 300, 110625.	1.7	6
13	Comprehensive characterization of mainstream marijuana and tobacco smoke. Scientific Reports, 2020, 10, 7160.	1.6	51
14	A novel protocol for producing low-abundance targets to characterize the sensitivity limits of ignitable liquid detection canines. Forensic Chemistry, 2020, 18, 100230.	1.7	5
15	Retention and release of odorants in cotton and polyester fabrics following multiple soil/wash procedures. Textile Reseach Journal, 2020, 90, 2212-2222.	1.1	9
16	Thermodynamics-based retention maps to guide column choices for comprehensive multi-dimensional gas chromatography. Analytica Chimica Acta, 2019, 1086, 133-141.	2.6	13
17	Thermodynamicsâ€based modelling of gas chromatography separations across column geometries and systems, including the prediction of peak widths. Journal of Separation Science, 2019, 42, 2013-2022.	1.3	11
18	A simple, fast, and accurate thermodynamic-based approach for transfer and prediction of GC retention times between columns and instruments Part II: Estimation of target column geometry. Journal of Separation Science, 2018, 41, 2553-2558.	1.3	7

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19	A simple, fast, and accurate thermodynamicâ€based approach for transfer and prediction of gas chromatography retention times between columns and instruments Part I: Estimation of reference column geometry and thermodynamic parameters. Journal of Separation Science, 2018, 41, 2544-2552.	1.3	14
20	A simple, fast, and accurate thermodynamicâ€based approach for transfer and prediction of gas chromatography retention times between columns and instruments Part III: Retention time prediction on target column. Journal of Separation Science, 2018, 41, 2559-2564.	1.3	11
21	Total Ion Spectra versus Segmented Total Ion Spectra as Preprocessing Tools for Gas Chromatography â€“ Mass Spectrometry Data. Journal of Forensic Sciences, 2018, 63, 1059-1068.	0.9	11
22	Modern Instrumental Limits of Identification of Ignitable Liquids in Forensic Fire Debris Analysis. Separations, 2018, 5, 58.	1.1	9
23	Synthetic Clothing and the Problem With Odor. Clothing and Textiles Research Journal, 2018, 36, 251-266.	2.2	14
24	Comprehensive two-dimensional gas chromatographic profiling and chemometric interpretation of the volatile profiles of sweat in knit fabrics. Analytical and Bioanalytical Chemistry, 2017, 409, 1905-1913.	1.9	20
25	Local Ion Signatures (LIS) for the examination of comprehensive two-dimensional gas chromatography applied to fire debris analysis. Forensic Chemistry, 2017, 3, 1-13.	1.7	19
26	Estimation of start and stop numbers for cluster resolution feature selection algorithm: an empirical approach using null distribution analysis of Fisher ratios. Analytical and Bioanalytical Chemistry, 2017, 409, 6699-6708.	1.9	10
27	The analysis of alkyl phosphates in nitrogen-rich crude oils using GC Ã— GC-NPD with a polar/apolar column configuration. Analytical Methods, 2017, 9, 5301-5309.	1.3	5
28	Disentangling Structural Confusion through Machine Learning: Structure Prediction and Polymorphism of Equiatomic Ternary Phases ABC. Journal of the American Chemical Society, 2017, 139, 17870-17881.	6.6	73
29	Indole-3-Acetic Acid Is Produced by Emiliania huxleyi Coccolith-Bearing Cells and Triggers a Physiological Response in Bald Cells. Frontiers in Microbiology, 2016, 7, 828.	1.5	63
30	Classifying Crystal Structures of Binary Compounds AB through Cluster Resolution Feature Selection and Support Vector Machine Analysis. Chemistry of Materials, 2016, 28, 6672-6681.	3.2	76
31	Determination of Hydrocarbon Group-Type of Diesel Fuels by Gas Chromatography with Vacuum Ultraviolet Detection. Analytical Chemistry, 2016, 88, 5809-5817.	3.2	59
32	The influence of temperature on the pyrolysis of household materials. Journal of Analytical and Applied Pyrolysis, 2016, 118, 75-85.	2.6	9
33	Thermodynamic-based retention time predictions of endogenous steroids in comprehensive two-dimensional gas chromatography. Analytical and Bioanalytical Chemistry, 2015, 407, 4091-4099.	1.9	15
34	Axillary odour build-up in knit fabrics following multiple use cycles. International Journal of Clothing Science and Technology, 2014, 26, 274-290.	0.5	27
35	Chemometric classification of casework arson samples based on gasoline content. Forensic Science International, 2014, 235, 24-31.	1.3	41
36	Rapid determination of thermodynamic parameters from one-dimensional programmed-temperature gas chromatography for use in retention time prediction in comprehensive multidimensional chromatography. Journal of Chromatography A, 2014, 1325, 204-212.	1.8	17

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37	Profiling Alkyl Phosphates in Industrial Petroleum Samples by Comprehensive Two-Dimensional Gas Chromatography with Nitrogen Phosphorus Detection (GC Ã— GCâ€“NPD), Post-column Deans Switching, and Concurrent Backflushing. Energy & Fuels, 2014, 28, 1709-1716.	2.5	8
38	Quantitative structureâ€“retention relationship modeling of gas chromatographic retention times based on thermodynamic data. Journal of Chromatography A, 2014, 1358, 225-231.	1.8	6
39	Unique Ion Filter: A Data Reduction Tool for GC/MS Data Preprocessing Prior to Chemometric Analysis. Analytical Chemistry, 2014, 86, 7726-7733.	3.2	20
40	A standardized method for the calibration of thermodynamic data for the prediction of gas chromatographic retention times. Journal of Chromatography A, 2014, 1330, 69-73.	1.8	16
41	Application of thermodynamic-based retention time prediction to ionic liquid stationary phases. Journal of Separation Science, 2014, 37, 1460-1466.	1.3	6
42	Gas chromatographic retention of alkyl phosphates on ionic liquid stationary phases. Journal of Chromatography A, 2013, 1271, 170-175.	1.8	14
43	Three-dimensional cluster resolution for guiding automatic chemometric model optimization. Talanta, 2013, 103, 252-259.	2.9	16
44	Comprehensive multidimensional separations for the analysis of petroleum. Journal of Chromatography A, 2012, 1255, 12-23.	1.8	61
45	Integration parameters and their effects on quantitative results with two-step peak summation quantitation in comprehensive two-dimensional gas chromatography. Journal of Chromatography A, 2012, 1255, 190-195.	1.8	9
46	Limits of Detection and Quantification in Comprehensive Multidimensional Separations. 1. A Theoretical Look. Analytical Chemistry, 2012, 84, 6646-6653.	3.2	12
47	Analysis of alkyl phosphates in petroleum samples by comprehensive two-dimensional gas chromatography with nitrogen phosphorus detection and post-column Deans switching. Journal of Chromatography A, 2012, 1252, 171-176.	1.8	19
48	Prediction of retention times in comprehensive two-dimensional gas chromatography using thermodynamic models. Journal of Chromatography A, 2012, 1255, 184-189.	1.8	34
49	Considerations for the automated collection of thermodynamic data in gas chromatography. Journal of Separation Science, 2012, 35, 2228-2232.	1.3	10
50	Cluster resolution: A metric for automated, objective and optimized feature selection in chemometric modeling. Talanta, 2011, 83, 1079-1087.	2.9	35
51	Study of alkyl phosphates in industrial petroleum mixtures by comprehensive two-dimensional gas chromatography time-of-flight mass spectrometry. Analytical and Bioanalytical Chemistry, 2011, 401, 2415-2422.	1.9	13
52	Using GC Ã— GC-FID profiles to estimate the age of weathered gasoline samples. Analytical and Bioanalytical Chemistry, 2011, 401, 2423-2431.	1.9	17
53	Comprehensive multidimensional separations. Analytical and Bioanalytical Chemistry, 2011, 401, 2333-2334.	1.9	2
54	Automated optimization and construction of chemometric models based on highly variable raw chromatographic data. Analytica Chimica Acta, 2011, 697, 8-15.	2.6	26

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55	Influence of carrier gas on the prediction of gas chromatographic retention times based on thermodynamic parameters. Journal of Chromatography A, 2011, 1218, 3241-3246.	1.8	14
56	Estimation of the age of a weathered mixture of volatile organic compounds. Analytica Chimica Acta, 2011, 694, 31-37.	2.6	33
57	One-pot microwave derivatization of target compounds relevant to metabolomics with comprehensive two-dimensional gas chromatography. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2010, 878, 1761-1770.	1.2	37
58	Prediction of gas chromatographic retention time via an additive thermodynamic model. Journal of Chromatography A, 2010, 1217, 4862-4867.	1.8	42
59	Methodology for the derivatization and quantification of dialkyl phosphate esters in petroleum samples. Analytical Methods, 2010, 2, 1176.	1.3	9
60	Comparison of peak integration methods for the determination of enantiomeric fraction in environmental samples. Chemosphere, 2009, 75, 1042-1048.	4.2	41
61	Excel Tutorial: Using the Least-Squares Method To Calculate Unknown Concentrations and Error. Journal of Chemical Education, 2009, 86, 879.	1.1	0
62	Modulation-induced error in comprehensive two-dimensional gas chromatographic separations. Journal of Chromatography A, 2008, 1200, 17-27.	1.8	30
63	Comprehensive two-dimensional gas chromatography for the separation of fatty acids in milk. European Journal of Lipid Science and Technology, 2007, 109, 757-766.	1.0	35
64	Modulation Ratio in Comprehensive Two-dimensional Gas Chromatography. Analytical Chemistry, 2006, 78, 4578-4587.	3.2	148
65	Fast GCÃ—GC with Short Primary Columns. Analytical Chemistry, 2006, 78, 2028-2034.	3.2	28
66	Comparison of column phase configurations for comprehensive two dimensional gas chromatographic analysis of crude oil and bitumen. Organic Geochemistry, 2006, 37, 1190-1194.	0.9	59
67	Effect of first-dimension column film thickness on comprehensive two-dimensional gas chromatographic separation. Journal of Chromatography A, 2006, 1105, 17-24.	1.8	15
68	Comparison of comprehensive two-dimensional gas chromatography in conventional and stop-flow modes. Journal of Chromatography A, 2006, 1105, 159-167.	1.8	24
69	Separation of technical 4-nonylphenols and their biodegradation products by comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry. Journal of Chromatography A, 2006, 1107, 233-239.	1.8	37
70	Identification of isomeric 4-nonylphenol structures by gas chromatographyâ€“tandem mass spectrometry combined with cluster analysis. Journal of Chromatography A, 2006, 1102, 245-255.	1.8	36
71	Evaluation of New Stationary Phases for the Separation of Fatty Acid Methyl Esters. Chromatographia, 2006, 63, S61-S66.	0.7	42
72	Projection of multidimensional GC data into alternative dimensionsâ€”exploiting sample dimensionality and structured retention patterns. Analytical and Bioanalytical Chemistry, 2006, 386, 602-613.	1.9	22

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73	Evaluation of New Stationary Phases for the Separation of Fatty Acid Methyl Esters. Chromatographia, 2006, 63, S61.	0.7	1
74	Overloading of the second-dimension column in comprehensive two-dimensional gas chromatography. Journal of Chromatography A, 2005, 1071, 21-27.	1.8	39
75	Flow model for coupled-column gas chromatography systems. Journal of Chromatography A, 2005, 1086, 135-140.	1.8	29
76	Comprehensive two-dimensional gas chromatography in stop-flow mode. Journal of Separation Science, 2004, 27, 431-441.	1.3	49
77	The evolution of comprehensive two-dimensional gas chromatography (GCÃ—GC). Journal of Separation Science, 2004, 27, 359-379.	1.3	169
78	New liquid nitrogen cryogenic modulator for comprehensive two-dimensional gas chromatography. Journal of Chromatography A, 2003, 1019, 53-63.	1.8	73
79	Design considerations for a GCÃ—GC system. Journal of Separation Science, 2002, 25, 304-310.	1.3	25
80	Design considerations for a GCÃ—GC system. , 2002, 25, 304.		1
81	Hydrothermal aging of polyimide film. Journal of Applied Polymer Science, 0, , 52183.	1.3	5