## Ludovic Duponchel

List of Publications by Year in descending order

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84 papers

2,317 citations

218677 26 h-index 243625 44 g-index

86 all docs

86 docs citations

86 times ranked 2739 citing authors

| #  | Article   | IF           | CITATIONS |
|----|---|--------------|-----------|
| 1  | Support vector machines (SVM) in near infrared (NIR) spectroscopy: Focus on parameters optimization and model interpretation. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 27-33.             | 3.5          | 211       |
| 2  | Simultaneous data pre-processing and SVM classification model selection based on a parallel genetic algorithm applied to spectroscopic data of olive oils. Food Chemistry, 2014, 148, 124-130.              | 8.2          | 104       |
| 3  | Resolution and segmentation of hyperspectral biomedical images by Multivariate Curve<br>Resolution-Alternating Least Squares. Analytica Chimica Acta, 2011, 705, 182-192.                                   | 5.4          | 100       |
| 4  | The Organization Pattern of Root Border-Like Cells of Arabidopsis Is Dependent on Cell Wall<br>Homogalacturonan   Â. Plant Physiology, 2009, 150, 1411-1421.  | 4.8          | 94        |
| 5  | Classification of edible fats and oils by principal component analysis of Fourier transform infrared spectra. Food Chemistry, 1996, 57, 245-251.  | 8.2          | 86        |
| 6  | Comparison of supervised pattern recognition methods with McNemar's statistical test. Analytica Chimica Acta, 2003, 477, 187-200.   | 5.4          | 83        |
| 7  | Exploration of megapixel hyperspectral LIBS images using principal component analysis. Journal of Analytical Atomic Spectrometry, 2018, 33, 210-220.  | 3.0          | 67        |
| 8  | Metal-induced malformations in early Palaeozoic plankton are harbingers of mass extinction. Nature Communications, 2015, 6, 7966.   | 12.8         | 66        |
| 9  | Multivariate Curve Resolution Methods in Imaging Spectroscopy:  Influence of Extraction Methods and Instrumental Perturbations. Journal of Chemical Information and Computer Sciences, 2003, 43, 2057-2067. | 2.8          | 63        |
| 10 | Monitoring polymorphic transformations by using in situ Raman hyperspectral imaging and image multiset analysis. Analytica Chimica Acta, 2014, 819, 15-25.  | 5.4          | 63        |
| 11 | Topological data analysis: A promising big data exploration tool in biology, analytical chemistry and physical chemistry. Analytica Chimica Acta, 2016, 910, 1-11.  | 5.4          | 59        |
| 12 | In-line and real-time prediction of recombinant antibody titer by inÂsitu Raman spectroscopy. Analytica Chimica Acta, 2015, 892, 148-152.   | 5.4          | 58        |
| 13 | Quality Evaluation of Sugar Beet(Beta vulgaris) by Near-Infrared Spectroscopy. Journal of Agricultural and Food Chemistry, 2004, 52, 1055-1061.   | 5.2          | 56        |
| 14 | Characterisation of heavy oils using near-infrared spectroscopy: Optimisation of pre-processing methods and variable selection. Analytica Chimica Acta, 2011, 705, 227-234.                                 | 5.4          | 54        |
| 15 | Parallel genetic algorithm co-optimization of spectral pre-processing and wavelength selection for PLS regression. Chemometrics and Intelligent Laboratory Systems, 2011, 107, 50-58.                       | 3 <b>.</b> 5 | 47        |
| 16 | Classification of challenging Laser-Induced Breakdown Spectroscopy soil sample data - EMSLIBS contest. Spectrochimica Acta, Part B: Atomic Spectroscopy, 2020, 169, 105872.                                 | 2.9          | 47        |
| 17 | Comparability of Raman Spectroscopic Configurations: A Large Scale Cross-Laboratory Study.<br>Analytical Chemistry, 2020, 92, 15745-15756.  | 6.5          | 46        |
| 18 | Chemometric Strategies To Unmix Information and Increase the Spatial Description of Hyperspectral Images: A Single-Cell Case Study. Analytical Chemistry, 2013, 85, 6303-6311.                              | 6.5          | 43        |

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|----|---|-----|-----------|
| 19 | Multivariate statistical process control (MSPC) using Raman spectroscopy for in-line culture cell monitoring considering time-varying batches synchronized with correlation optimized warping (COW). Analytica Chimica Acta, 2017, 952, 9-17. | 5.4 | 42        |
| 20 | Statistical tests for comparison of quantitative and qualitative models developed with near infrared spectral data. Journal of Molecular Structure, 2003, 654, 253-262.   | 3.6 | 36        |
| 21 | Pushing back the limits of Raman imaging by coupling super-resolution and chemometrics for aerosols characterization. Scientific Reports, 2015, 5, 12303.   | 3.3 | 35        |
| 22 | Detection of minor compounds in complex mineral samples from millions of spectra: A new data analysis strategy in LIBS imaging. Analytica Chimica Acta, 2020, 1114, 66-73.  | 5.4 | 32        |
| 23 | Super-resolution and Raman chemical imaging: From multiple low resolution images to a high resolution image. Analytica Chimica Acta, 2008, 607, 168-175.  | 5.4 | 30        |
| 24 | Combination of mid-infrared spectroscopy and chemometric factorization tools to study the oxidation of lubricating base oils. Catalysis Today, 2010, 155, 255-260.  | 4.4 | 30        |
| 25 | Classification of Green Coffees by FT-IR Analysis of Dry Extract. Applied Spectroscopy, 1995, 49, 580-585.  | 2.2 | 29        |
| 26 | Time-Resolved Step-Scan FT-IR Spectroscopy:  Focus on Multivariate Curve Resolution. Journal of Chemical Information and Computer Sciences, 2003, 43, 1966-1973.  | 2.8 | 27        |
| 27 | Quantitative analysis of latex in paper coatings by ATR-FTIR spectroscopy. Journal of Chemometrics, 1994, 8, 333-347.   | 1.3 | 26        |
| 28 | A Cell Wall Proteome and Targeted Cell Wall Analyses Provide Novel Information on Hemicellulose<br>Metabolism in Flax. Molecular and Cellular Proteomics, 2017, 16, 1634-1651.  | 3.8 | 23        |
| 29 | Developing global regression models for metabolite concentration prediction regardless of cell line.<br>Biotechnology and Bioengineering, 2017, 114, 2550-2559.   | 3.3 | 23        |
| 30 | Chemometric strategies for the study of the complexation of Al(III) ions with model molecule of humic substances from UV–vis data sets. Analytica Chimica Acta, 2005, 544, 337-344.   | 5.4 | 22        |
| 31 | Trappist beer identification by vibrational spectroscopy: A chemometric challenge posed at the †Chimiomà ©trie 2010 †congress. Chemometrics and Intelligent Laboratory Systems, 2012, 113, 2-9.   | 3.5 | 22        |
| 32 | Gaussian mixture models for the classification of highâ€dimensional vibrational spectroscopy data. Journal of Chemometrics, 2010, 24, 719-727.  | 1.3 | 21        |
| 33 | Exploring hyperspectral imaging data sets with topological data analysis. Analytica Chimica Acta, 2018, 1000, 123-131.  | 5.4 | 20        |
| 34 | Infrared chemical imaging: Spatial resolution evaluation and super-resolution concept. Analytica Chimica Acta, 2010, 674, 220-226.  | 5.4 | 19        |
| 35 | Water quality assessment of a small peri-urban river using low and high frequency monitoring. Environmental Sciences: Processes and Impacts, 2016, 18, 624-637.   | 3.5 | 19        |
| 36 | Neural network modelling for very small spectral data sets: reduction of the spectra and hierarchical approach. Chemometrics and Intelligent Laboratory Systems, 2000, 54, 93-106.  | 3.5 | 18        |

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|----|---|-----|-----------|
| 37 | Highly sensitive terahertz spectroscopy in microsystem. RSC Advances, 2012, 2, 10064.   | 3.6 | 18        |
| 38 | Multivariate curve resolution of step-scan FTIR spectral data. Vibrational Spectroscopy, 2004, 35, 21-26.   | 2.2 | 16        |
| 39 | Fast epi-detected broadband multiplex CARS and SHG imaging of mouse skull cells. Biomedical Optics Express, 2018, 9, 245.   | 2.9 | 16        |
| 40 | Insights from Nitrogen Compounds in Gas Oils Highlighted by High-Resolution Fourier Transform Mass Spectrometry. Analytical Chemistry, 2019, 91, 12644-12652.   | 6.5 | 16        |
| 41 | UDP-GLYCOSYLTRANSFERASE 72E3 Plays a Role in Lignification of Secondary Cell Walls in Arabidopsis. International Journal of Molecular Sciences, 2020, 21, 6094.   | 4.1 | 16        |
| 42 | Mammalian cell culture monitoring using <i>in situ</i> spectroscopy: Is your method really optimised?. Biotechnology Progress, 2017, 33, 308-316.   | 2.6 | 15        |
| 43 | Multi-excitation hyperspectral autofluorescence imaging for the exploration of biological samples.<br>Analytica Chimica Acta, 2019, 1062, 47-59.  | 5.4 | 15        |
| 44 | Data fusion of LIBS and PIL hyperspectral imaging: Understanding the luminescence phenomenon of a complex mineral sample. Analytica Chimica Acta, 2022, 1192, 339368.   | 5.4 | 15        |
| 45 | Quantitative determination of polymer and mineral content in paper coatings by infrared spectroscopy. Improvements by non-linear treatments. Analytica Chimica Acta, 1996, 335, 79-85.                              | 5.4 | 13        |
| 46 | Hydrolysis of hemoglobin surveyed by infrared spectroscopy. Analytica Chimica Acta, 1999, 396, 241-251.   | 5.4 | 13        |
| 47 | Should we prefer inverse models in quantitative LIBS analysis?. Journal of Analytical Atomic Spectrometry, 2020, 35, 794-803.   | 3.0 | 13        |
| 48 | Increasing the spatial resolution of near infrared chemical images (NIR-CI): The super-resolution paradigm applied to pharmaceutical products. Chemometrics and Intelligent Laboratory Systems, 2012, 117, 183-188. | 3.5 | 12        |
| 49 | Tracking hidden organic carbon in rocks using chemometrics and hyperspectral imaging. Scientific Reports, 2018, 8, 2396.  | 3.3 | 12        |
| 50 | Chemometric Exploration of APPI(+)-FT-ICR MS Data Sets for a Comprehensive Study of Aromatic Sulfur Compounds in Gas Oils. Analytical Chemistry, 2019, 91, 11785-11793.   | 6.5 | 12        |
| 51 | Effect of image processing constraints on the extent of rotational ambiguity in MCR-ALS of hyperspectral images. Analytica Chimica Acta, 2019, 1052, 27-36.   | 5.4 | 12        |
| 52 | Matrix merging arrangements for the study protein dynamics by time-resolved step-scan Fourier transform infrared spectroscopy and multivariate curve resolution. Analytica Chimica Acta, 2004, 515, 183-190.        | 5.4 | 11        |
| 53 | New chemometric approach MCR-ALS to unmix EPR spectroscopic data from complex mixtures. Journal of Magnetic Resonance, 2014, 248, 27-35.  | 2.1 | 11        |
| 54 | Fusing spectral and spatial information with 2-D stationary wavelet transform (SWT 2-D) for a deeper exploration of spectroscopic images. Talanta, 2021, 224, 121835.   | 5.5 | 11        |

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|----|---|-----|-----------|
| 55 | Interpretation and improvement of an artificial neural network MIR calibration. Chemometrics and Intelligent Laboratory Systems, 2002, 62, 189-198.   | 3.5 | 10        |
| 56 | Combination of mid-infrared spectroscopy and curve resolution method to follow the antioxidant action of alkylated diphenylamines. Chemometrics and Intelligent Laboratory Systems, 2011, 106, 210-215.                       | 3.5 | 10        |
| 57 | Combining near and mid infrared spectroscopy for heavy oil characterisation. Fuel, 2014, 133, 310-316.  | 6.4 | 10        |
| 58 | Studying radiolytic ageing of nuclear power plant electric cables with FTIR spectroscopy. Talanta, 2017, 172, 139-146.  | 5.5 | 10        |
| 59 | Coherent anti-Stokes Raman scattering under electric field stimulation. Physical Review B, 2016, 94, .  | 3.2 | 9         |
| 60 | Neighbouring pixel data augmentation: a simple way to fuse spectral and spatial information for hyperspectral imaging data analysis. Journal of Chemometrics, 2017, 31, e2882.  | 1.3 | 9         |
| 61 | Low-Level Fusion of Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Data Sets for the Characterization of Nitrogen and Sulfur Compounds in Vacuum Gas Oils. Analytical Chemistry, 2020, 92, 2815-2823.            | 6.5 | 9         |
| 62 | Towards a new pseudo-quantitative approach to evaluate the ionization response of nitrogen compounds in complex matrices. Scientific Reports, 2021, 11, 6417.   | 3.3 | 9         |
| 63 | Extraction of Pure Spectral Signatures and Corresponding Chemical Maps from EPR Imaging Data Sets: Identifying Defects on a CaF <sub>2</sub> Surface Due to a Laser Beam Exposure. Analytical Chemistry, 2015, 87, 3929-3935. | 6.5 | 8         |
| 64 | Topological data analysis (TDA) applied to reveal pedogenetic principles of European topsoil system. Science of the Total Environment, 2017, 586, 1091-1100.  | 8.0 | 8         |
| 65 | Detection of formaldehyde oxidation catalysis by MCR-ALS analysis of multiset ToF-SIMS data in positive and negative modes. Chemometrics and Intelligent Laboratory Systems, 2017, 171, 80-85.                                | 3.5 | 8         |
| 66 | Image Fusion. Data Handling in Science and Technology, 2019, , 311-344.   | 3.1 | 8         |
| 67 | Angle Distribution of Loading Subspace (ADLS) for estimating chemical rank in multivariate analysis: Applications in spectroscopy and chromatography. Talanta, 2019, 194, 90-97.  | 5.5 | 8         |
| 68 | Sulfur compounds characterization using FT-ICR MS: Towards a better comprehension of vacuum gas oils hydrodesulfurization process. Fuel Processing Technology, 2020, 210, 106529.   | 7.2 | 8         |
| 69 | Archaeological Mortar Characterization Using Laser-Induced Breakdown Spectroscopy (LIBS) Imaging Microscopy. Applied Spectroscopy, 2022, , 000370282110711.   | 2.2 | 8         |
| 70 | Randomised SIMPLISMA: Using a dictionary of initial estimates for spectral unmixing in the framework of chemical imaging. Talanta, 2020, 217, 121024.   | 5.5 | 7         |
| 71 | When remote sensing meets topological data analysis. Journal of Spectral Imaging, 0, , .  | 0.0 | 7         |
| 72 | Has your ancient stamp been regummed with synthetic glue? A FT-NIR and FT-Raman study. Talanta, 2016, 149, 250-256.   | 5.5 | 6         |

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|----|--|--------------|-----------|
| 73 | Determination of the Reactivity Degree of Various Alkaline Solutions: A Chemometric Investigation. Applied Spectroscopy, 2019, 73, 1361-1369.  | 2.2          | 6         |
| 74 | A detailed analysis of the influence of $\hat{l}^2$ -cyclodextrin derivates on the thermal denaturation of lysozyme. International Journal of Pharmaceutics, 2019, 554, 1-13.  | 5.2          | 6         |
| 75 | Robust variable selection in the framework of classification with label noise and outliers: Applications to spectroscopic data in agri-food. Analytica Chimica Acta, 2021, 1153, 338245.   | 5.4          | 6         |
| 76 | Degree of hydrolysis from mid-infrared spectra. Analytica Chimica Acta, 2001, 446, 255-266.  | 5.4          | 5         |
| 77 | Exploration of the Reactivity of Heteroatomic Compounds Contained in Vacuum Gas Oils during Hydrotreatment Using Fourier Transform Ion Cyclotron Resonance Mass Spectrometry. Energy & Energy Fuels, 2020, 34, 10752-10761.  | 5.1          | 5         |
| 78 | Saturated signals in spectroscopic imaging: why and how should we deal with this regularly observed phenomenon?. Analytica Chimica Acta, 2021, 1157, 338389.   | 5.4          | 4         |
| 79 | New strategy to identify radicals in a time evolving EPR data set by multivariate curve resolution-alternating least squares. Analytica Chimica Acta, 2016, 947, 9-15.   | 5.4          | 3         |
| 80 | Second-order universal calibration. Talanta, 2020, 212, 120787.  | 5 <b>.</b> 5 | 3         |
| 81 | Novel four-dimensional approach for the structural characterization of neutral nitrogen compounds in vacuum gas oils using UHPLC-IM-QqToF analysis. Analytica Chimica Acta, 2021, 1169, 338611.  | 5.4          | 3         |
| 82 | Evaluating the Benefits of Data Fusion and PARAFAC for the Chemometric Analysis of FT-ICR MS Data Sets from Gas Oil Samples. Energy & Ener | 5.1          | 2         |
| 83 | Super-Resolution in Vibrational Spectroscopy. Data Handling in Science and Technology, 2016, 30, 477-517.  | 3.1          | 1         |
| 84 | Complete determination of plant tissues based only on autoâ€fluorescence and the advanced image analysis – study of needles and stamens. Journal of Chemometrics, 2015, 29, 521-527.   | 1.3          | 0         |