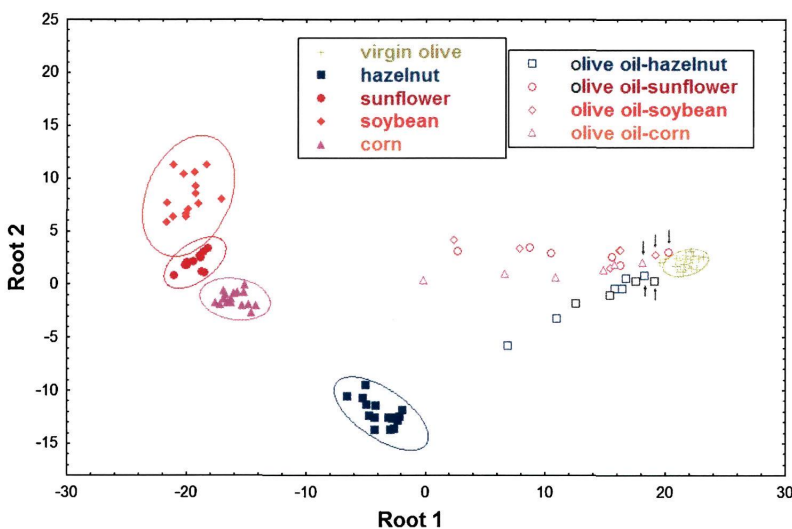


ANALYTICA CHIMICA ACTA

AN INTERNATIONAL JOURNAL DEVOTED TO ALL BRANCHES OF ANALYTICAL CHEMISTRY



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Review Article

Quality assessment and authentication of virgin olive oil by NMR spectroscopy: A critical review

Photis Dais and Emmanuel Hatzakis

(Published on pp. 1-27 of this issue)

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Editorial Board

Page iii

Review articles

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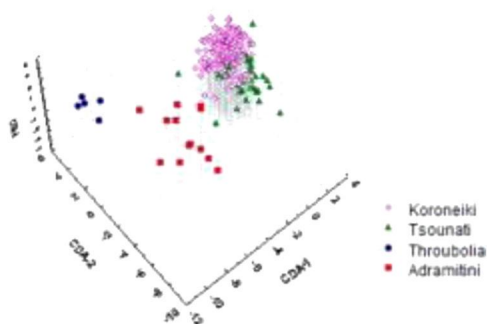
Quality assessment and authentication of virgin olive oil by NMR spectroscopy: A critical review

Review Article

Pages 1-27

Photis Dais, Emmanuel Hatzakis

Graphical abstract



Highlights

► Overview of olive oil analysis by ^1H , ^{13}C , and ^{31}P NMR spectroscopy. ► Sample preparation. ► Experimental conditions and processing for metabonomic analysis. ► Multivariate statistical methods for NMR data analysis. ► Quality assessment and authentication of extra virgin olive oil.

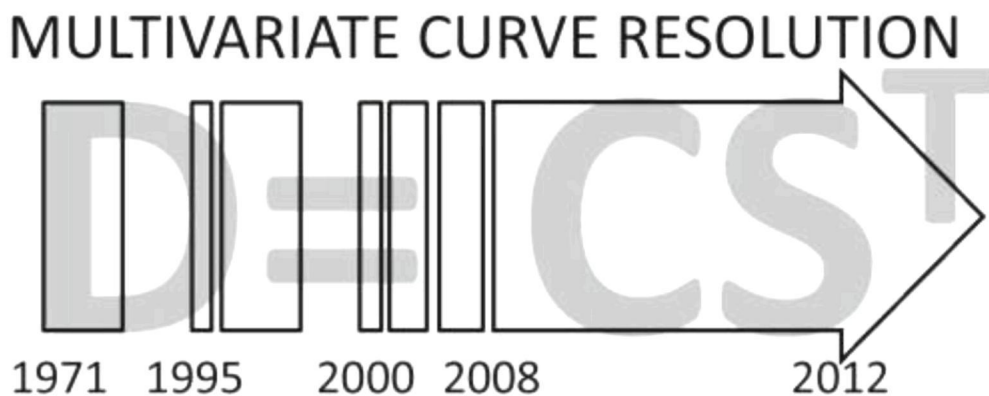
3

Multivariate curve resolution: A review of advanced and tailored applications and challenges

Review Article

Pages 28-36

Graphical abstract



Highlights

► MCR is nowadays a well-established and widespread methodology for mixture analysis. ► The analytical issues requiring advanced applications of MCR are reviewed. ► Attention is paid to the literature published the years 2008–2012.

Chemometrics

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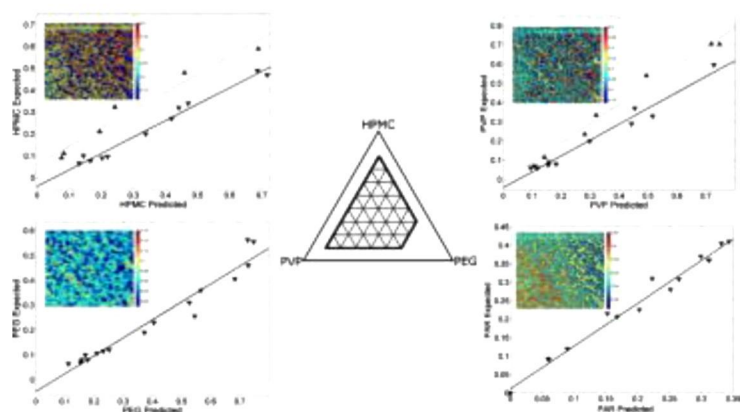
NIR imaging spectroscopy for quantification of constituents in polymers thin films loaded with paracetamol

Original Research Article

Pages 37-44

Guilherme L. Alexandrino, Ronei J. Poppi

Graphical abstract



Highlights

► NIR chemical imaging and chemometrics were used for studying thin films based drug delivery systems. ► Thin films were polymers mixtures of HPMC, PVP and PEG-400 loaded with the drug paracetamol. ► MCR-ALS provided initial biased results on quantification of polymers and additional calibration step was required. ► Three different strategies were tested to suppress the bias on the quantification by MCR-ALS. ► Paracetamol distribution in the thin films has direct correlation with the PVP and PEG, but inverse correlation with HPMC.

5

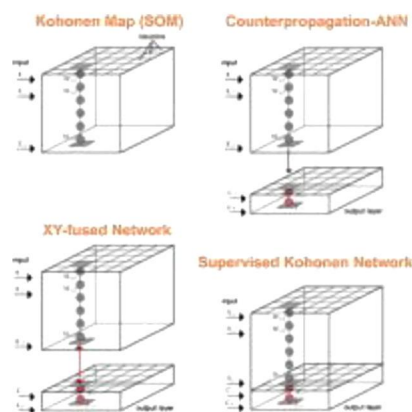
Effects of supervised Self Organising Maps parameters on classification performance

Original Research Article

Pages 45-53

Davide Ballabio, Mahdi Vasighi, Peter Filzmoser

Graphical abstract



Highlights

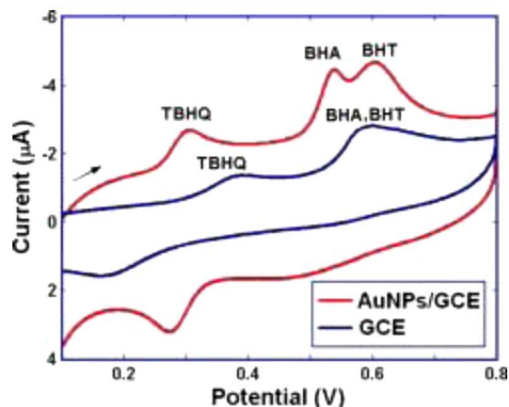
► We evaluated effects of SOMs parameters on classification and computational time. ► The study was conducted on eighteen real datasets. ► Significant parameters and their interactions on classification were highlighted. ► Optimal architectures to reduce the computational time of SOMs was proposed.

Electrochemistry

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Glassy carbon electrodes modified with gold nanoparticles for the simultaneous determination of three food antioxidants

Graphical abstract



Highlights

- ▶ A gold nanoparticles modified glassy carbon electrode (AuNPs/GCE) was constructed.
- ▶ The electrochemical mechanism of BHA, BHT and TBHQ at the AuNPs/GCE was studied.
- ▶ The oxidation products of BHA and TBHQ were found to be the same.
- ▶ First-derivative method was used to resolve the overlapped voltammograms.
- ▶ Synthetic antioxidants in food samples were analyzed.

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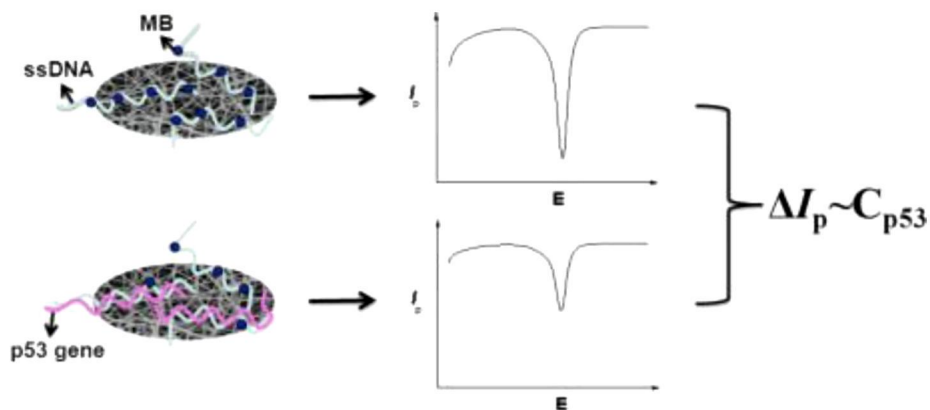
Novel electrochemical biosensor based on functional composite nanofibers for sensitive detection of p53 tumor suppressor gene

Original Research Article

Pages 63-69

Xiaoying Wang, Xiaobing Wang, Xiaoning Wang, Fentian Chen, Kehui Zhu, Qian Xu, Meng Tang

Graphical abstract



Highlights

- ▶ A novel electrochemical p53 biosensor based on functional composite nanofibers (MWNTs–PA6–PPy) was developed.
- ▶ The MWNTs–PA6–PPy electrode with large specific surface area and good biocompatibility can be used to enhance stability, speed and sensitivity.
- ▶ The biosensor can detect 50 fM wild type p53 sequence.
- ▶ The strategy could be extended to develop various sensors for the detection of many kinds of analytes.

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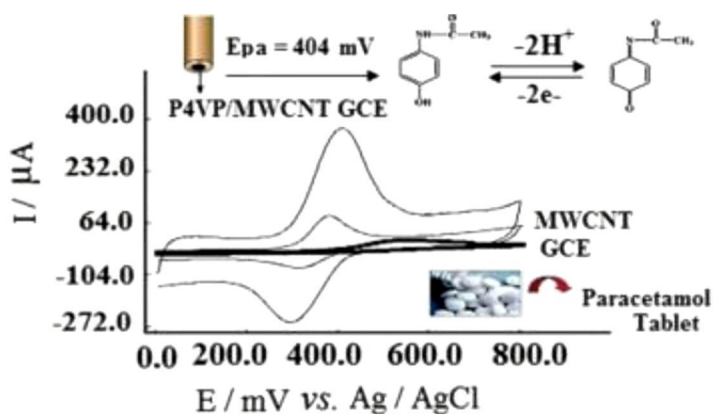
Sensitive voltammetric determination of paracetamol by poly (4-vinylpyridine)/multiwalled carbon nanotubes modified glassy carbon electrode

Original Research Article

Pages 70-76

Hanieh Ghadimi, Ramin M.A.Tehrani, Abdussalam Salhin Mohamed Ali, Norita Mohamed, Sulaiman Ab Ghani

Graphical abstract



Highlights

► A P4VP/MWCNT modified glassy carbon electrode was fabricated and characterized. ► The electrode was useful for determination of paracetamol. ► At optimum conditions, ascorbic acid and uric acid did not interfere in the electrode activity. ► The electrode exhibited good sensitivity, reproducibility and stability. ► The electrode was used for the determination of paracetamol in formulation tablets and urine samples.

Mass Spectrometry

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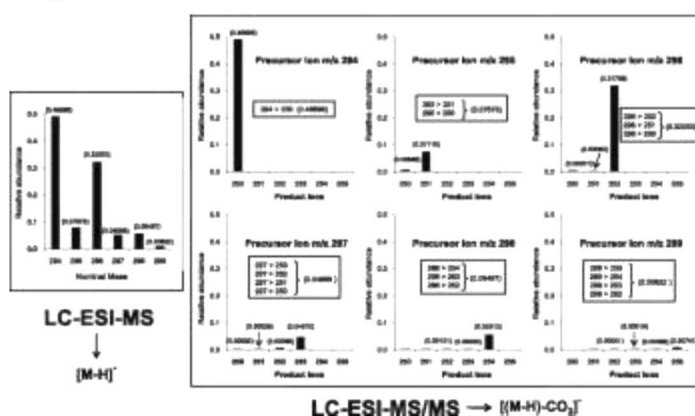
Isotope pattern deconvolution-tandem mass spectrometry for the determination and confirmation of diclofenac in wastewaters

Original Research Article

Pages 77-85

Ángel Castillo, Emma Gracia-Lor, Antoni Francesc Roig-Navarro, Juan Vicente Sancho, Pablo Rodríguez-González, J. Ignacio García Alonso

Graphical abstract



Highlights

► Isotope dilution with isotope pattern deconvolution (IPD) has been applied to LC-MS/MS. ► The procedure allows the determination of organic compounds without calibration graph. ► Diclofenac determination in wastewater showed the need of this methodology in LC-MS/MS. ► Confirmation was accomplished with routine transitions used in multiresidue analysis. ► IPD permits the minimal labeling of the analyte which minimizes isotopic effect.