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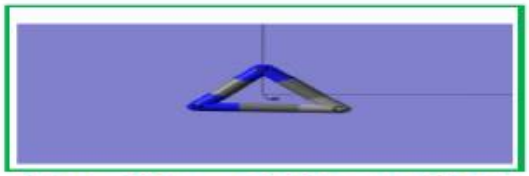
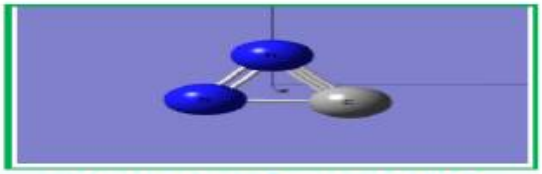
(International Peer Reviewed Journal)

New Chemistry News

$^{-}N=C=N^{-}$



New News of Chem (NNC)



ChemNewsNew (CNN)

3-way data in

Omnimetrics

Information Source (is)
ACS.org
Sciencedirect.com

Omnimetrics

1. **Medicinometrics**
2. **Dietetometrics**
3. **Environmetrics**
4. **Methodo Metrics**

1. Medicinometrics

Chem.Syst:

Antiparkinson agents
- Levodopa (LDP)
- Carbidopa (CDP)
- Methyldopa (MDP)
- Benserazide (BA)
- Tolcapone (TOL)
- Entacapone (ENT) + dopamine (DPA) as uncalibrated interference

Sample.RealLife.Environment
- Antiparkinson agents

Instrument
- Differential pulse voltammetric (DPV)

Complexity. Sample
- Presence of uncalibrated interference

Data.Measurement
- Generation of second-order data at different pulse heights

Methods.MathStat:
- MCR-ALS
- PARAFAC2

Method. reference
- HPLC-UV)

Method. MathStat	Data Processing
Asymmetric least square spline regression (ASLSSR) Correlation optimized warping (COW)	Corrected recorded data for ▪ Baseline ▪ Potential shift

Method. Calib.	Capability
Three-way calibration model	Predict analytes' concentrations in absence and presence of DPA
MCR-ALS	Results better than PARAFAC2

Exploiting second-order advantage from mathematically modeled voltammetric data for simultaneous determination of multiple antiparkinson agents in the presence of uncalibrated interference

Journal of the Taiwan Institute of Chemical Engineers, 88(2018)49-61
doi.org/10.1016/j.jtice.2018.04.007

GhobadMohammadi and Khodabakhsh Rashidi and Majid Mahmoudi and Hector C. Goicoechea and Ali R. Jalalvand

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Thiamine

Sample.RealLife.Environment
- Multivitamin complexes

Instrument
- Ex.Em.Fl.

Data.Measurement
- Kinetic-fluorescent

Methods.MathStat:
- PARAFAC

Method. Chemometric

- Thiamine (vitamin B1) was converted into a fluorescent thiochrome by oxidation catalyzed by Hg2+ in alkaline medium\
- The kinetic evolution of conversion was monitored by emission-excitation spectroscopy
- Output: Third-Order Dataset for each sample Or four-way data array for a group of samples

- Second-order advantage does not prevent
  - Matrix effects or
  - Interferences.

✓ Remedy: standard addition method →
✓ Develops into a quantitative method

Chemometric modeling of kinetic-fluorescent third-order data for thiamine determination in multivitamin complexes

Microchemical Journal, 128(2016)42-46
doi.org/10.1016/j.microc.2016.04.006

Wallace D. Fragoso and Alejandro C. Olivieri

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- Naphazoline hydrochloride
- Pyridoxine hydrochloride

Sample.RealLife.Environment

- Eye drops

Complexity. Sample

- Interferences
  - Unknown
  - Uncalibrated

Instrument

- Ex.Em.Fl.

Advntages

+ High sensitivity
+ Low-cost
+ Simple implementation

Method. Confirmation

- Multiple reaction monitoring (MRM) by
  - LC–MS/MS method.

Simultaneous determination of naphazoline and pyridoxine in eye drops using excitation–emission matrix fluorescence coupled with second-order calibration method based on alternating trilinear decomposition algorithm

Chinese Chemical Letters, 26(2015)1446-1449
doi.org/10.1016/j.cclet.2015.07.015

Hui Xia and Hai-Long Wu and Hui-Wen Gu and Xiao-Li Yin and Huan Fang and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- Paracetamol
- Caffeine
- Sodium diclofenac

Experimental Design

- Central Composite

Instrument

- Spectrophotometer with ultraviolet (UV) detector (first order data)

Data.acquisition

- Calibration curves are built one for each analyte, like in univariate calibration
- Individual curves were grouped in a calibration matrix
- Curve of the analyte of interest was used for calibration

Methods.MathStat:

- MCR-ALS
- PLS

Order. Advantages

Instrum, First Order

Second Order advantage achieved by grouping first order profiles

\+ NO need to prepare mixtures of the analytes for calibration

A simplified and versatile multivariate calibration procedure for multiproduct quantification of pharmaceutical drugs in the presence of interferences using first order data and chemometrics

Microchemical Journal, 146(2019)202-209
doi.org/10.1016/j.microc.2019.01.014

Licarion Pinto and FranciellyStechi and Márcia Cristina Breitkreitz

Chem.Syst:

- Acetaminophen

Sample.RealLife.Environment

! Novafen samples

\

Complexity. Sample

- Unknown interferences

Data.Measured

- Spectroelectrochemical data

Data.Management

- augmentation mode : [Spectral ; kinetic]

Methods.MathStat:

- Matrix-augmentation multivariate curve resolution–alternating least-squares (MA-MCR–ALS)

MCR–ALS

\+ Flexible in applying trilinearity constraint for each component

\+ Makes it possible to manage deviations from trilinearity of data effectively

PARAFAC

\+ Full trilinear models

\- Not flexible to apply trilinearity in specific dimensions

MA-MCR–ALS

\+ Second order advantage achieved in solution of analytical task

Traditional Chinese medicines (TCM)

Chem.Syst:
- Umbelliferone
- Scopoletin

Sample.RealLife.Environment

Tibetan medicine
- Saussurealaniceps

Traditional Chinese medicine
- Radix angelicaepubescentis

Task.Chem.
- Estimation

Instrument
- Ex.Em.Fl
- HPLC-DAD

Complexity. Sample
- Presence of potential interferents

Methods.MathStat:
- Alternating trilinear decomposition (ATLD)

Chemometric advantagr
- Second-order advantage, hence simple pretreatment
- Use of “mathematical separation” instead of harsh (non-green) “physical or chemical separation”

Comparison of methods
- Ex.Em.Fl>> HPLC-DAD

Simultaneous determination of umbelliferone and scopoletin in Tibetan medicine Saussurealaniceps and traditional Chinese medicine Radix angelicaepubescentis using excitation-emission matrix fluorescence coupled with second-order calibration method

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 170(2017)104-110doi.org/10.1016/j.saa.2016.07.018

Li Wang and Hai-Long Wu and Xiao-Li Yin and Yong Hu and Hui-Wen Gu and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Nephrotoxic aristolochic acid I (AA-I)
- Aristololactam I (AL-I)

Sample.RealLife.Environment
- Chinese herbal medicines

Methods.MathStat: second-order.Calib
- Alternating penalty trilinear decomposition (APTLD)
- Self-weighted alternating trilinear decomposition (SWATLD)

Methods.Validation:
- LC-MS/MS

Method. Chem

→ Chemical derivatization that converts the non-fluorescent AA-I to high-fluorescent AL-I,

Interference-free spectrofluorometric quantification of aristolochic acid I and aristololactam I in five Chinese herbal medicines using chemical derivatization enhancement and second-order calibration methods

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 175(2017)229-238 doi.org/10.1016/j.saa.2016.12.030

Yong Hu and Hai-Long Wu and Xiao-Li Yin and Hui-Wen Gu and Rong Xiao and Li Wang and Huan Fang and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Herbs
- Volatile/heat-labile components in Ligusticum chuanxiong Hort–Cyperusrotundus rhizomes.

Sample.RealLife.Environment
- Traditional Chinese medicines

Instrument
- Head Space/Solid Phase Micro-Extraction (HS-SPME) coupled with Gas Chromatography/Mass Spectrometer (GC/MS)
- The retention time (RT) shift with multi-channel detection signals for different samples is vital to maintain trilinear structure

Methods.MathStat:	
Modified multiscale peak alignment (mMSPA) ▪ Continuous Wavelet Transform with Haar wavelet as the mother wavelet	Detects peak position and peak width of representative ion profile
Fast. Fourier Transform (FFT) cross correlation calculation	Confirmation of raw shift
Haar CWT	Arriving at optimal shift

A modified multiscale peak alignment method combined with trilinear decomposition to study the volatile/heat-labile components in Ligusticum chuanxiong Hort - Cyperusrotundus rhizomes by HS-SPME-GC/MS

Journal of Chromatography B, 1079(2018)41-50
doi.org/10.1016/j.jchromb.2018.01.040

Min He and Pan Yan and Zhi-Yu Yang and Zhi-Min Zhang and Tian-Biao Yang and Liang Hong

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- α-asarone
- β-asarone

Sample.RealLife.Environment

Complex Traditional Chinese medicine
- ! Acorustatarinowii

Data.Measurement

[Em-Fl matrices]

Complexity. Sample
- Unexpected interferents

\

Chemometric approach

Mmathematical separation
- \+ Physical or chemical separation step was avoided

Methods.MathStat:

Second-order calibration methods

- PARAFAC
- Alternating trilinear decomposition (ATLD)
- Alternating penalty trilinear decomposition (APTLD)
- Self-weighted alternating trilinear decomposition (SWATLD)

- Unfolded partial least-squares (U-PLS)
- Multidimensional partial least-squares (N-PLS) with residual bilinearization (RBL)

Simultaneous determination of α-asarone and β-asarone in Acorustatarinowii using excitation-emission matrix fluorescence coupled with chemometrics methods	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 191(2018)195-202 doi.org/10.1016/j.saa.2017.10.011
Xue-Mei Bai and Tie Liu and De-Long Liu and Yong-Ju Wei	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

$$$

Chem.Syst:

- Scopoletin
- Scopolin

Sample.RealLife.Environment

- ErycibeobtusifoliaBenth

Task.Chem.

- Quality control of traditional Chinese medicine (TCM)

Instrument	Task.Chem.Q(uality) C(ontrol)
Ex.Em.fl	Simultaneous quantification
Time-resolved (lifetimes) fluorescence	Qualitative identification

Complexity. Sample

- Significant spectral overlapping among analytes
- Interferences

Methods.MathStat:

- PARAFAC

Method. Reference

- HPLC-FLD

Time-resolved fluorescence and chemometrics-assisted excitation–emission fluorescence for qualitative and quantitative analysis of scopoletin and scopolin in ErycibeobtusifoliaBenth	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 219(2019)96-103 doi.org/10.1016/j.saa.2019.04.019
Tie Liu and Xin-Ge Li and Ji-Ye Wang and De-Long Liu and Yong-Ju Wei	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Veterinary drugs

Chem.Syst:	
21 Veterinary drugs	
1) Trimethoprim (TMP) **2)** Enrofloxacin (ENR) **3)** Imidacloprid (IMD) **4)** Clenbuterol (CLB) **5)** Difloxacin (DIF) **6)** Ceftiofur (CFT) **7)** Chloramphenicol(CAP) **8)** Chlortetracycline (CTC) **9)** Flumequine (FLU) **10)** Prednisolone (PSL) **11)** Pyrantel (PYR)	**1)** Menbutone (MBT) **2)** Albendazole (ABZ) **3)** Flunixin (FXN) **4)** Diazepam (DZP) **5)** Fenbendazole(FBZ) **6)** Nicarbazin (marker residue NN′-bis(4-nitrophenyl)urea) **7)** Diclofenac (DCF) **8)** Ibuprofen (IBU) **9)** Betamethasone (BMV) **10)** Progesterone (PGN)

Sample.RealLife.Environment
! Poultry industry
! livestock production
! livestock in Argentina

Methods.MathStat:
o MCR-ALS

Instrument:	Detector	Response
o HPLC o Chemstation software package (Agilent Technologies, Waldbronn, Germany) o To control the instrument, data acquisition and data analysis.	o Fast-scan fluorescence detection(FSFD)	o Intensity
	o Diode array detection (DAD)	o Absorbance

Exptaldsign
o Simplex-centroid design ▪ With combinations of MeOH, ACN (extracting mixture); ▪ sodium phosphate buffer
➔ To maximize the resolution of the analytes.

Data.Measurement
[Em-Fl matrices]

Uv-Vis Spectral range nm	Elution time period min	Data Matrix elution time x spectral dimensions
200-to-500	0.0-to-25.0	1868 × 151

Time-emission fluorescence data matrices (TEM)	
Spectral range (nm)	elution time period (min)
310 and 600	0.0 to 25.0
with the excitation wavelength fixed at 280	

Complexity. Data profile. chromatogram
- Baseline/background contributions
- Low signal-to-noise ratios (s/n)
- Elution time shifts
- Peak overlaps
Complexity. Samples
- Unexpected compounds
- Interferents

Simultaneous multi-residue determination of twenty one veterinary drugs in poultry litter by modeling three-way liquid chromatography with fluorescence and absorption detection data	Talanta, 167(2017)442-452doi.org/10.1016/j.talanta.2017.02.030
Carla M. Teglia and Paola M. Peltzer and Silvia N. Seib and Rafael C. Lajmanovich and María J. Culzoni and Héctor C. Goicoechea	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Cancer

Chem.Syst:
o Multiple breast cancer-related DNAs

DataSets
o Simulated example
o Analytical experiment
o Molecular beacons used for the simultaneous assay of three breast cancer related DNA targets
Output
+ Automatic estimation of number of components
+ Resolution of
o Spectral profile
o Concentration estimation

Complexity. Response
o Spectral overlap
Complexity. Response data. structure
o Lower (not full) rank

Methods.MathStat:

- Alternating residual trilinearization (ART)

\+ Automatic rank estimation for second-order calibration data tensor

\+ Avoids risk of chemically meaningless fitting of component spectra

Limitations.TLD

\- Parallel factor analysis (PARAFAC) requires a prior rank estimation

Remedy

✓ Alternating residual trilinearization (ART)

\+ Robust second-order calibration strategy for complex spectral analysis in multiplex fluorescence assays

A novel algorithm for second-order calibration of three-way data in fluorescence assays of multiple breast cancer-related DNAs

Talanta, 195(2019)433-440
doi.org/10.1016/j.talanta.2018.11.076

Lin Tan and Yan Zhang and Qin Yang and Nan Chen and Wen Du and Li-Juan Tang and Jian-Hui Jiang and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way--3way--3way-3way--3way--3way--3way--3way

Clinical Analysis

Chem.Syst:

Fluoroquinolones
- Moxifloxacin
- Ciprofloxacin

Sample.RealLife.Environment
- Urine

Instrument
- Ex.Em.Fl.

Methods.MathStat:
- PARAFAC
- SWATLD
- U-PLS/RBL

FOM
- Prediction (RMSEP)
- Recovery
- Elliptical joint confidence region (EJCR) plots

On the performance of multiway methods for simultaneous quantification of two fluoroquinolones in urine samples by fluorescence spectroscopy and second-order calibration strategies

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 136(2015)618-624
doi.org/10.1016/j.saa.2014.09.075

Maryam Vosough and Sara NoroozieEshlaghi and Reza Zadmard

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Norepinephrine (NE)
- Paracetamol (AC)
- Uric acid (UA)

\+

- Uncalibrated interference
  - Pteroylglutamic acid

Sample.RealLife. Environment
- Human serum

Complexity. Data.Instum.Chromat

Three-way arrays
- Non-bilinear
- Non-trilinear

Preproessing
- Observed shifts in the recorded DPV data were corrected using
  - Correlation optimised warping (COW) algorithm

Methods.MathStat:

- Artificial neural network-residual bilinearization (ANN-RBL)
- Unfolded-partial least squares-RBL (U-PLS/RBL)
- Multidimensional-partial least squares-RBL (N-PLS/RBL)
- Multivariate curve resolution-alternating least squares (MCR-ALS)
- Parallel factor analysis 2 (PARAFAC2)

Generation of non-multilinear three-way voltammetric arrays by an electrochemically oxidized glassy carbon electrode as an efficient electronic device to achieving second-order advantage: Challenges, and tailored applications	Talanta, 134(2015)607-618 doi.org/10.1016/j.talanta.2014.11.066
Ali R. Jalalvand and Mohammad-Bagher Gholivand and Hector C. Goicoechea and Thomas Skov	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- 2-hydroxy-4-methoxybenzophenone

Sample.RealLife.Environment

- Mice serum
- Human plasma

Instrument

- Ultra- HPLC

Complexity. Sample

- \- Coelution of BP-3 with the matrix components
- ✓ Resolved through second-order advantage of multi-way calibration

Methods.MathStat:

- MCR-ALS

Determination of 2-hydroxy-4-methoxybenzophenone in mice serum and human plasma by ultra-high-performance liquid chromatography enhanced by chemometrics	Microchemical Journal, 148(2019)35-41 doi.org/10.1016/j.microc.2019.04.032
Carla M. Teglia and Clarisa G. Santamaría and Horacio A. Rodriguez and María J. Culzoni and Héctor C. Goicoechea	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- Benzodiazepines
- Alprazolam
- Clonazepam
- Diazepam

Sample.RealLife.Environment

- Human serum

Complexity. Sample

- Uncalibrated components in the sample
  - Presence of serum endogenous components

Complexity. Response.Instrument

- Presence of overlapped profiles

Instrument

- HPLC-photodiode-array detection

Matrix-free analysis of selected benzodiazepines in human serum samples using alternating trilinear decomposition modeling of fast liquid chromatography diode array detection data	Talanta, 148(2016)454-462 doi.org/10.1016/j.talanta.2015.10.088
Maryam Vosough and Negar J. Iravani	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:	Sample.RealLife.Environment	Task.Chem.
o Phenanthrene metabolites	▪ Human breast milk ▪ Semi-skimmed commercial cow milk	▶ Quantitation

Instrument	Methods.MathStat:
o Ex.Em.Fl.	o n-way PLS o Unfolded PLS o N-PLS-Residual bilinearization (/RBL) o U-PLS/RBL o MCR-ALS

	Data.Aquisition
Steep 0	Optimized the chromatographic parameters, in isocratic mode (elution time 5.5 min)
Step 1	Second-order data (Elution time-emission fluorescence)

	Range	Units
Exciting	[250] Fixed	nm
Emission	[330 to 430; Inc: 1]	nm
Elution time	[0 to 5.5 ; Inc: 5.4 sec].	Min

Step 2

Validation samples	
1-, 2-, 3- and 4-Hydroxyphenanthrene	[1.0 to 9.0] ng mL−1
9-Hydroxyphenanthrene	[5.0 to 45.0] ng mL−1

Phenanthrene metabolites determination in human breast and cow milk by combining elution time-emission fluorescence data with multiway calibration	Talanta, 188(2018)299-307 doi.org/10.1016/j.talanta.2018.05.096
Elísabet Martín Tornero Anunciación Espinosa-Mansilla and Arsenio Muñoz de la Peña and Isabel Durán Merás	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Immunosuppressant drugs
- Tacrolimus
- Everolimus
- Cyclosporine A

Sample.RealLife.Environment
- Whole blood samples

Instrument
- Fast HPLC-DAD

Complexity. Sample

Non-calibrated blood components
- Chromatographic profiles
- Background drift
- Shifts
- Co-elution

✓ Resolved
- Background correction
  - ▶ MCR/ALS

Advantages

FigureOfMerit
- Increased selectivity
- Sensitivity
- Sufficiency of lower limit of quantification
- Simplicity of sample treatment steps
- Low-cost instrumentation compared with LC–MS/MS

Development of a fast HPLC-DAD method for simultaneous quantitation of three immunosuppressant drugs in whole blood samples using intelligent chemometrics resolving of coeluting peaks in the presence of blood interferences	Journal of Chromatography B, 1073(2018)69-79

doi.org/10.1016/j.jchromb.2017.12.012

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Adenosine

Sample.RealLife.Environment
- Urinary adenosine

Task.Chem.

Diagnosis
- ▶ Non-invasive monitoring of cancer

Instrument
- Surface-enhanced Raman spectroscopy

Methods.MathStat:
- ▶ MCR-ALS

Method. Chemometric
- Standard addition method
- pH controls

were combined
- \+ Compensate for the matrix effect
- \+ To address overlapping bands in the analysis of human urine samples

Adenosine
- Adenosine is a purine nucleoside present in all human cells
- Essential in regulating physiological activities in tissues and organs
- Potential cancer biomarker in urine
  - \+ Crucial for the early diagnosis
  - \+ Non-invasive monitoring clinical analysis

Surface-enhanced Raman spectroscopy and MCR-ALS for the selective sensing of urinary adenosine on filter paper	Talanta, 187(2018)99-105 doi.org/10.1016/j.talanta.2018.05.022

Javier E.L. Villa and CelioPasquini and Ronei J. Poppi

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- Uric acid
- Creatinine
- Tyrosine
- Homovanillic acid
- Hippuric acid
- Indole-3-acetic acid
- Tryptophan
- 2-methylhippuric acid)

Sample.RealLife.Environment

- Human urine

Instrument

- HPLC-DAD

Complexity. Data

Chromatograms
- Highly overlapping peaks
- Distortions in the time and baseline

Analytes
- Presence of interferences
  - Unknown
  - Background

Advantages

- \+ Increased selectivity, sensitivity
- \+ Shorter analysis time
- \+ Undemanding elution conditions
- \+ Sufficiency of lower limit of quantification
- \+ Second order advantages

.

Method. Validation

- Classic HPLC

Methods.MathStat:

- ATLD
- MCR-ALS

Target-based metabolomics for fast and sensitive quantification of eight small molecules in human urine using HPLC-DAD and chemometrics tools resolving of highly overlapping peaks

Talanta, 201(2019)174-184
doi.org/10.1016/j.talanta.2019.03.090

Xiao-Dong Sun and Hai-Long Wu and Zhi Liu and Yue Chen and Jun-Chen Chen and Li Cheng and Yu-Jie Ding and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

vinca alkaloids
- Vincristine (VCR)
- Vinblastine (VLB)
- Vindoline (VDL)
- Catharanthine (CAT)
- Yohimbine (YHB)

Sample.RealLife.Environment

- Catharanthus roseus
- Human serum

Instrument

- HPLC_DAD

Complexity. Data

Instrumental profiles
- Presence of heavy overlaps
- Interferences i.e. .Analytes not present in calibration set

Methods.MathStat:

- Alternating trilinear decomposition
- Trilinear component modeling

Rapid and simultaneous determination of five vinca alkaloids in Catharanthus roseus and human serum using trilinear component modeling of liquid chromatography–diode array detection data	Journal of Chromatography B, 1026(2016)114-123 doi.org/10.1016/j.jchromb.2015.08.008
Zhi Liu and Hai-Long Wu and Yong Li and Hui-Wen Gu and Xiao-Li Yin and Li-Xia Xie and Ru-Qin Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst: Drugs o Gliclazide o Glibenclamide o Glimepiride o Atenolol o Enalapril o Amlodipine	Sample.RealLife.Environment ! Serum samples Instrument o HPLC-UV o EmFl
Multiway calibration strategy with chromatographic data exploiting the second-order advantage for quantitation of three antidiabetic and three antihypertensive drugs in serum samples	Microchemical Journal, 136(2018)185-192 doi.org/10.1016/j.microc.2016.11.019
Celina M. Monzón and Carla M. Teglia and Mario R. Delfino and Héctor C. Goicoechea	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

2. Dietetometrics

Chem.Syst:
- o Grape harvest

Sample.RealLife.Environment
- ▪ Red grapes from four different varieties,in sixteen representative (in both geographical and edaphic point of view) plots belonging to the Qualified Designation of Origin (DOC) Rioja.

Task.Chem.

Analysis of effect of the spatial and temporal distribution on physicochemical profile of the grape
- o Grape quality
- o Maturation
- o Qualified Designation of Origin Rioja
- o Variability among vineyards

Data.3way
1) Sample (plot/variety) 16

Parameters
2) Physicochemical 12
3) Temporal

Methods.MathStat:
- ▶ PARAFAC

Parallel factor analysis for monitoring data from a grape harvest in Qualified Designation of Origin Rioja including spatial and temporal variability	Chemometrics and Intelligent Laboratory Systems, 146(2015)347-353 doi.org/10.1016/j.chemolab.2015.06.003
E. Meléndez and L.A. Sarabia and M.C. Ortiz	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- o Allura red (AR)
- o Sunset yellow (SY)

Sample.RealLife.Environment
- ▪ Model compounds in
  - ▪ soft drinks
  - ▪ food samples

Instrument
- o HPLC-UV

Complexity. Data.Response
- o Severe spectral overlapping between the AR and SY
- ➔ Strong collinearities

Methods. Limitation. MVC. second-order
- o PARAFAC
- o MCR-ALS
  - - Not successful if collinearities

Methods.MathStat:
- ▶ Bilinear least squares/residual bilinearization (BLLS/RBL)
- \+ Easy sample pretreatment
- \+ Accuracy
- \+ Sufficient spectral resolution
- \+ Concentration prediction

Robust to
- \+ Presence of unknown interferences
- \+ Strongly overlapping spectra
- \+ Collinearities problems

Application of bilinear least squares/residual bilinearization in bulk liquid membrane system for simultaneous multicomponent quantification of two synthetic dyes	Chemometrics and Intelligent Laboratory Systems, 144(2015)48-55 doi.org/10.1016/j.chemolab.2015.03.012
RouhollahKhani and Jahan B. Ghasemi and FarzanehShemirani and Reza Rahmanian	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- o Aflatoxins B1, B2

Sample.RealLife.Environment
- ▪ Peanuts

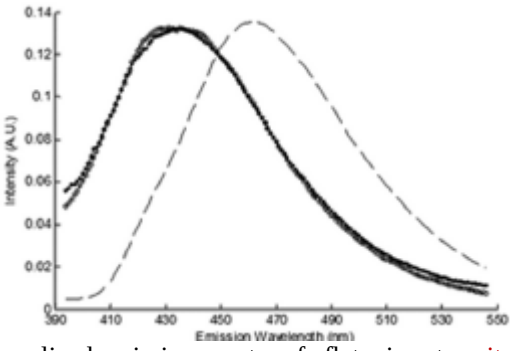
Instrument
- o Ex.Em.Fl

Complexity. Data.Instum.Chromat
- ▪ Rank overlap

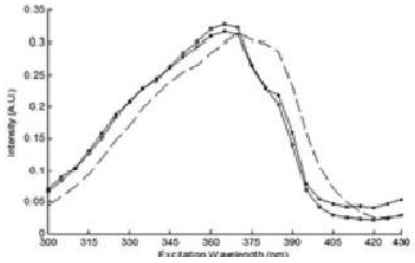
3rd Oder (4-way) Data Tensor:
- \+ Resurrecting second-order advantage

Knowledge Base Method. 3way-4way-Data & Order & MVC Methods
If there is rank overlap in one mode, **Then** 3-way algorithms : PARAFAC under some constraints resolve successfully
If a species has rank overlap in both modes of EEF data **Then i**nformation of the data matrix is equivalent to a zero-order data for that species **Example:.** Aflatoxins B1 and B2 have the same shape of spectral profiles in both excitation and emission modes
If solvent as a new additional selectivity mode is used **Then** EEF data with solvent becomes third order data for each sample **If** third order data, in turn, converted to the second order data by augmentation **Then** it resurrects second order advantage in original EEMs
If three-way data is constructed by stacking augmented data in the third way & analyzed by second order calibration methods (BLLS–RBL and PARAFAC) **Then** results of both are methods are good agreement **Example:**quantification of analytes in four kinds of peanut samples

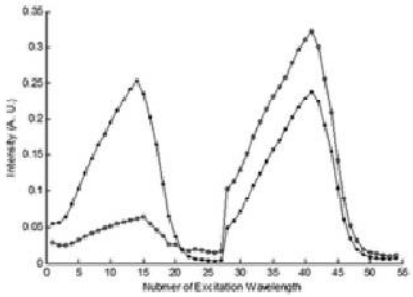
3way-080



Normalized emission spectra of aflatoxins at excitation peak of 360 nm:
AFB1 (6 ppb) -○-○-,
AFB2 (2 ppb) -*-*-, AFG2 (2 ppb) – –.\

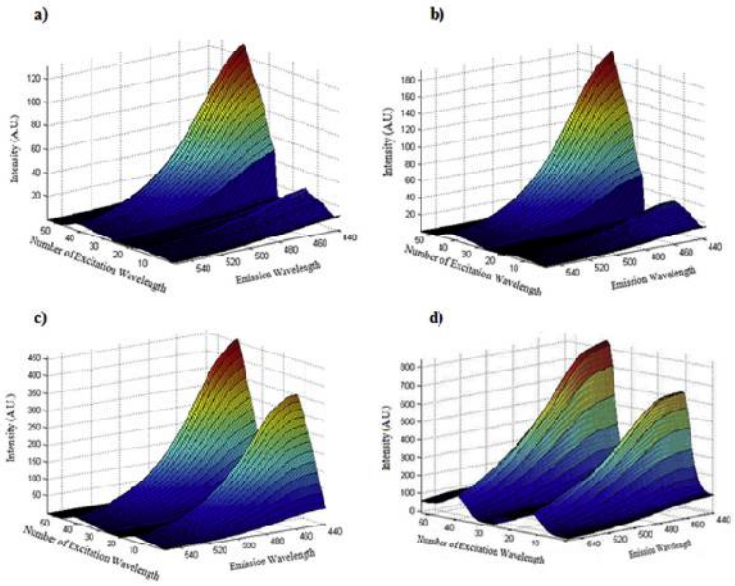


:
The normalized excitation spectra of aflatoxins at emission peak of 445 nm
AFB1 (6 ppb) -○-○-, AFB2 (2 ppb) -*-*-, AFG2 (2 ppb) – –.



Normalized augmented excitation spectra of

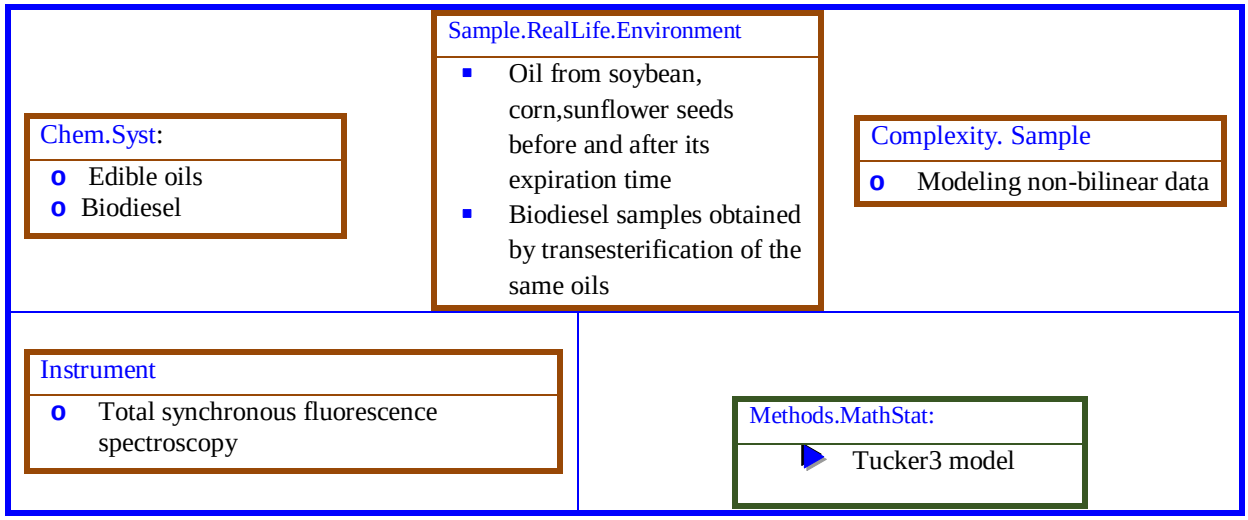
AFB1 (6 ppb) and
AFB2 (2 ppb)
In the absence/presence of β-cyclodextrin (AFB1 -○-○-, AFB2 -*-*-).



The augmented EEMs spectra of
(a) AFB1 (6 ppb), (b) AFB2 (2 ppb),
(c) the mixture of AFB1 (9 ppb) and AFB2 (3 ppb); and
(d) peanut 1 in the absence/presence of 0.01 M β-cyclodextrin.

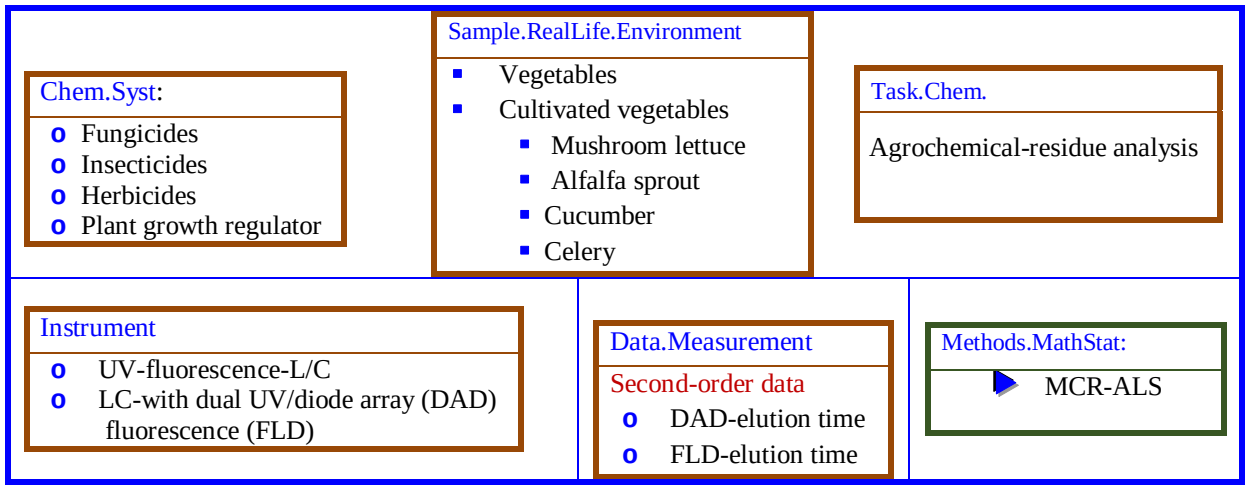
Quantifying aflatoxins in peanuts using fluorescence spectroscopy coupled with multi-way methods: Resurrecting second-order advantage in excitation–emission matrices with rank overlap problem	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 156(2016)63-69 doi.org/10.1016/j.saa.2015.11.022
S. Maryam Sajjadi and Hamid Abdollahi and Reza Rahmanian and Leila Bagheri	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way



Fluorescent fingerprints of edible oils and biodiesel by means total synchronous fluorescence and Tucker3 modeling	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 175(2017 doi.org/10.1016/j.saa.2016.12.027
MatíasInsausti and Adriano de Araújo Gomes and José Manuel Camiña and Mario Cesar Ugulino de Araújo and Beatriz Susana Fernández Band	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way



A green-analytical chemistry method for agrochemical-residue analysis in vegetables	Microchemical Journal, 128(2016)34-41 doi.org/10.1016/j.microc.2016.03.006
Maira D. Carabajal and Juan A. Arancibia and Graciela M. Escandar	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Methods.	Name	Purpose
Experimental	D-optimal design	Effect of four experimental factors on figures of merit
Instrumental	Excitation emission fluorescence matrix	Function relationship of Response data with concentration
Math.Modeling	Parallel factor analysis	Trilinear Fn relationship between Fl response of analyte and its Concentration

Migration test of Bisphenol A from polycarbonate cups using excitation-emission fluorescence data with parallel factor analysis

Talanta, 167(2017) 367-378
doi.org/10.1016/j.talanta.2017.02.033

M.L. Spagnuolo and F. Marini and L.A. Sarabia and M.C. Ortiz

Chem.Syst:
- Camellia oil

Sample.RealLife.Environment
- ! Adulterated with cheaper vegetable oil

Instrument
- Ex.Em-Fl spectrometer

Methods.MathStat:
PARAFAC

\

Method	Purpose
Classification	Two-directional two-dimensional LDA
n-PLS	Adulteration level in camellia oil

Rapid identification and quantification of cheaper vegetable oil adulteration in camellia oil by using excitation-emission matrix fluorescence spectroscopy combined with chemometrics

Food Chemistry, 293(2019)348-357
doi.org/10.1016/j.foodchem.2019.04.109

Tong Wang and Hai-Long Wu and Wan-Jun Long and Yong Hu and Li Cheng and An-Qi Chen and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Rhodamine dyes

Sample.RealLife.Environment
- Illegally added into chilli samples

Instrument
- Ex.Em.Fl.

Complexity. Sample
fluorescence spectra
- Scattering, peak overlaps
- Unknown interferences
  - Constant background
  - Different kinds of backgrounds

Methods.MathStat:
- ATLD

Melthod.Verification
- HPLC-FLD

Rapid, simultaneous and interference-free determination of three rhodamine dyes illegally added into chilli samples using excitation-emission matrix fluorescence coupled with second-order calibration method	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 204(2018)141-149 doi.org/10.1016/j.saa.2018.06.031
Yue-Yue Chang and Hai-Long Wu and Huan Fang and Tong Wang and Zhi Liu and Yang-Zi Ouyang and Yu-Jie Ding and Ru-Qin Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Synthetic colorants
- Tartrazin
- Sunset yellow

Sample.RealLife.Environment
- Adulterated saffron

Task.Chem.
- Quality assessment

Instrument
- Spectrophotometer

Complexity. Sample
- Rank deficiency in concentration mode impaired the system
- Remedy: Three-way variation array V was generated by subtracting the first pH spectrum from each spectrum at each pH

Quality assessment of the saffron samples using second-order spectrophotometric data assisted by three-way chemometric methods via quantitative analysis of synthetic colorants in adulterated saffron	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 148(2015)389-395 doi.org/10.1016/j.saa.2015.03.135
Saeed Masoum and Ali Gholami and MarjanHemmesi and Saleheh Abbasi	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Dyes
- Tartrazine
- Carminic acid

Sample.RealLife.Environment

foods --complex matrices
- Mustard
- Ketchup
- Asparagus soup powder
- Pumpkin soup powder
- Plum jam
- Orange-strawberry juice

Data.Measurement
- Kinetic-spectroscopic data

Methods.MathStat:
- Multivariate curve resolution

Multivariate curve resolution applied to kinetic-spectroscopic data matrices: Dye determination in foods by means of enzymatic oxidation	Talanta, 169(2017)189-194 doi.org/10.1016/j.talanta.2017.03.079
Valeria Boeris and Juan A. Arancibia and Alejandro C. Olivieri	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Weathered oils

Data.Measurement
- Infrared indexes

Methods.MathStat:
- Self-organizing maps

Data.dimensions
Oils × weathering aliquots × analytical variables

Differentiation of weathered oils using infrared indexes and self-organizing maps	Fuel, 158(2015)57-65 doi.org/10.1016/j.fuel.2015.04.064
M.P. Gómez-Carracedo and J.M. Andrade-Garda and D. Prada-Rodríguez	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst: o Capsaicin o Dihydrocapsaicin	Sample.RealLife.Environment ! Spicy foods	Instrument o HPLC–FLD o LC- Detector
Complexity. Sample - Profiles of capsaicin and dihydrocapsaicin (major capsaicinoids) are identical Solution: Results are only for total content of capsaicinoids	Data.Measurement [Ex.Em-Fl matrices]	Methods.MathStat second-order calibration ▪ PARAFAC ▪ U-PLS/RBL

Determination of pungency in spicy food by means of excitation-emission fluorescence coupled with second-order chemometric calibration	Journal of Food Composition and Analysis, 67(2018) 10-18 doi.org/10.1016/j.jfca.2017.12.031
Olga Monago-Maraña and María Guzmán-Becerra and Arsenio Muñoz de la Peña and Teresa Galeano-Díaz	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

$$$

Chem.Syst: o Malic, oxalic, formic, lactic, acetic, citric, pyruvic, succinic, tartaric, propionic, α-cetoglutaric acids	Sample.RealLife.Environment ▪ Dairy products (yoghurt, cultured milk ,cheese) ▪ Fermented food. ▪ Wine
Instrument o RP-HPLC-DAD	Methods.MathStat: (PARAFAC) U-PLS/RBL)
Multivariate analysis of organic acids in fermented food from reversed-phase high-performance liquid chromatography data	Talanta, 178(2018) 15-23 doi.org/10.1016/j.talanta.2017.09.005
Pablo Mortera and Federico A. Zuljan and Christian Magni and Santiago A. Bortolato and Sergio H. Alarcón	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Extra virgin olive oils

Task
- ! Classification

Instrument
LC-DAD

Data.Management
- Fusion of mean data profiles in both spectral and time domains.
  - ✓ PCA, PLS-DA,
  - ✓ SIMCA, NPLS-DA

RF method

Sensibility	1.0
Specificity	0.92
Accuracy	0.95

Methods.MathStat:
- MCR-ALS
- Random forest

Classification of olive oils according to their cultivars based on second-order data using LC-DAD

Talanta, 195(2019)69-76
doi.org/10.1016/j.talanta.2018.11.033

Ana M. Jiménez-Carvelo and Carlos M. Cruz and Alejandro C. Olivieri and Antonio González-Casado and Luis Cuadros-Rodríguez

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Vanillin

Sample.RealLife.Environment
Flavoring agent in
- Foods
- Pharmaceuticals

Task.Chem.
- To predict the pKa values

Data.Measurement
- Square wave voltammetric (SWV) technique

Three-dimensional (3-D) voltammetric plots
= Fn(potential (mV) and frequency (Hz))

Methods.MathStat:
- MCR-ALS
- PARAFAC

	#	Range
pHs	12	1.3–12.0
frequencies	8	5–120 Hz

A comparative application of two-way and three-way analysis to three-dimensional voltammetric dataset for the pKa determination of vanillin

Journal of Electroanalytical Chemistry, 826(2018)133-141
doi.org/10.1016/j.jelechem.2018.07.047

Zehra Yazan and SevcanErden and ErdalDinç

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Leucomalachite green
- Leucocrystal violet
- Their chromic forms

Sample.RealLife.Environment
- Fish and shrimp muscle

Instrument
- Ex.Em.Fl

Method. Comparison	Methods.MathStat:
o HPLC	▶ PARAFAC ▶ ATLD

Determination of leucomalachite green, leucocrystal violet and their chromic forms using excitation–emission matrix fluorescence coupled with second-order calibration after dispersive liquid–liquid microextraction

Food Chemistry, 185(2015)479-487
doi.org/10.1016/j.foodchem.2015.02.149

Saiqin Ju and Jian Deng and Jianlin Cheng and Ni Xiao and Kaihui Huang and Canhui Hu and Haiqing Zhao and JinXie and Xiaozhu Zhan

3way--3way--3way--3way--3way--3way--3way--3way--3way--3wa

Beverages

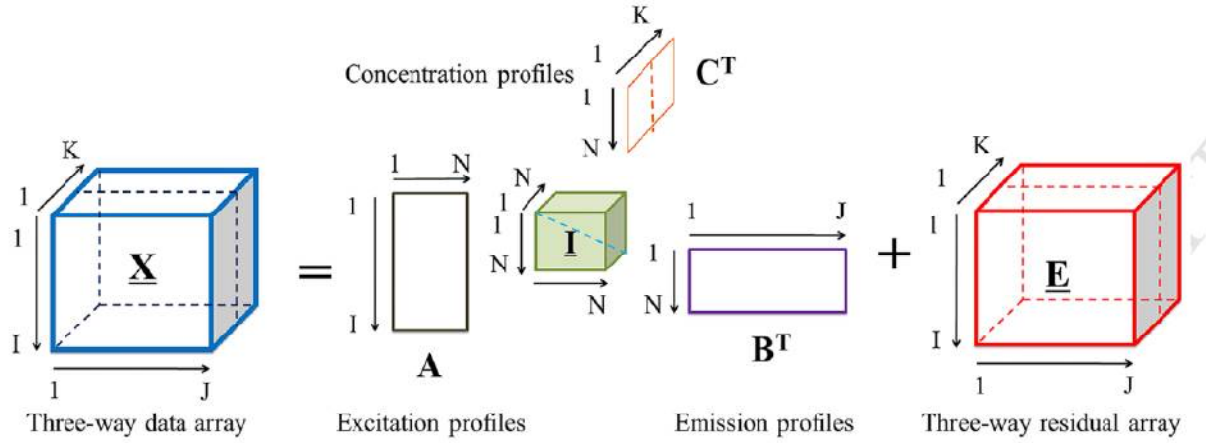
Chem.Syst:	Sample.RealLife.Environment	Task.Chem.
o Tea samples	o Tea varieties	▶ Classification

Methods.MathStat:	Method.	
▪ Alternating trilinear decomposition method + ▪ Two-dimensional LDA	Simulated data sets different levels of o Noise o Class overlap o Number of groups	o ATLD-2DLDA superior classification than o ATLD-LDA, o 2D-LDA o N-PLS-DA

Real data sets

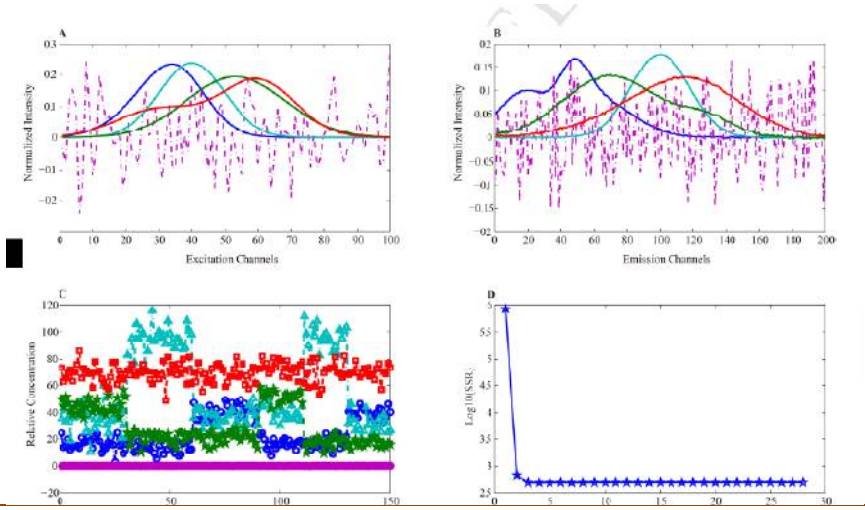
- o Chemically meaningful model
- o Characterizing different tea varieties
- o Best correct classification rate for test samples, (100%)

Methods.MathStat:	% success
ATLD-LDA	83.9
2D-LDA	90.3
N-PLS-DA	90.3.



Experimental 3-way = Mathematical tri-linear decomposition + unmodelled

$$x_{ijk} = \sum_{n=1}^{N} a_{in} b_{jn} c_{kn} + e_{ijk} \quad (i = 1, 2\ldots, I, j = 1, 2\ldots, J, k = 1, 2\ldots, K)$$



A flexible and novel strategy of alternating trilinear decomposition method coupled with two-dimensional linear discriminant analysis for three-way chemical data analysis: Characterization and classification	Analytica Chimica Acta, 1021(2018) doi.org/10.1016/j.aca.2018.03.050
Yong Hu and Hai-Long Wu and Xiao-Li Yin and Hui-Wen Gu and Zhi Liu and Rong Xiao and Li-Xia Xie and Huan Fang and Ru-Qin Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3wa

Chem.Syst:

Endocrine-disruptor
- Bisphenol A
- Nonylphenol
- Octylphenol
- Diethyl phthalate
- dibutyl phthalate
- Diethylhexyl phthalate

Sample.RealLife.Environment
- Beer, wine
- Soda, juice, water
- Distilled beverage

Data.Measurement
- Elution time-absorbance wavelength
- Elution time-fluorescence emission wavelength

Complexity. Response. Instruments
- Partially overlapped
  - Chromatographic profiles
  - Spectral bands

Complexity. samples
- Potential interferents

Methods.MathStat:
- MCR-ALS

Method. comparison
- GC-MS

A green method for the quantification of plastics-derived endocrine disruptors in beverages by chemometrics-assisted liquid chromatography with simultaneous diode array and fluorescent detection

Talanta, 159(2016)336-343
doi.org/10.1016/j.talanta.2016.06.049

Rocío B. Pellegrino Vidal and Gabriela A. Ibañez and Graciela M. Escandar

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Antidiabetic agents
  - Sulfonylurea-type

Sample.RealLife.Environment
- Health teas
- Human plasma samples

Complexity. Sample
- Unknown interferences

Instrument
- LC–MS
  Full scan mode

Methods.MathStat:
- ATLD

Chemometrics-enhanced full scan mode of liquid chromatography–mass spectrometry for the simultaneous determination of six co-eluted sulfonylurea-type oral antidiabetic agents in complex samples

Chemometrics and Intelligent Laboratory Systems, 155(2016)62-72
doi.org/10.1016/j.chemolab.2016.04.001

Hui-Wen Gu and Hai-Long Wu and Shan-Shan Li and Xiao-Li Yin and Yong Hu and Hui Xia and Huan Fang and Ru-Qin Yu and Peng-Yuan Yang and Hao-Jie Lu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Carbendazim

Sample.RealLife.Environment
- Orange juice

Task.Chem.
- Pseudo-univariate calibration based on independent component analysis (ICA)

Instrument
- NIR

Algorithm.

Input: NIR (900 to 1700nm)
- First derivative to baseline correction
- ICA + JADE (Joint Approximate Diagonalization of Eigenmatrices)

Complexity. Data.Instum.NIR ▪ Analyte with interferent	order – (second)- advantage ▪ Analyte with interferent **!! Higher order advantage with lower order instruments** ▪ Second order advantage with first order data achieved.
Pseudo-univariate calibration based on independent component analysis for determination of the carbendazim concentration in orange juice	Microchemical Journal, 134(2017)114-118 doi.org/10.1016/j.microc.2017.05.016
Géssica M. Ribeiro and Daniel A. Madivadua and Suzana M.M. Curti and Leonardo P. Pantean and Paulo Henrique Março and Patrícia Valderrama	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst: o Mycotoxins	Sample.RealLife.Environment o Moldy foods o Cereals
Instrument o LC-MS o Full scan-mass spectrometry	Methods.MathStat: o ATLD
Chemometrics-enhanced liquid chromatography-full scan-mass spectrometry for interference-free analysis of multi-class mycotoxins in complex cereal samples	Chemometrics and Intelligent Laboratory Systems, 160(2017)125-138 doi.org/10.1016/j.chemolab.2016.12.003
Zhi Liu and Hai-Long Wu and Li-Xia Xie and Yong Hu and Huan Fang and Xiao-Dong Sun and Tong Wang and Rong Xiao and Ru-Qin Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst: o Six synthetic colorants	Sample.RealLife.Environment ▪ Complex food sample ▪ Beverage
Complexity. Sample o HPLC-DAD	Instrument o HPLC-DAD
Methods.MathStat: ▶ ATLD	Method. Reference o HPLC-UV
Chemometrics-assisted high performance liquid chromatography-diode array detection strategy to solve varying interfering patterns from different chromatographic columns and sample matrices for beverage analysis	Journal of Chromatography A, 1435(2016)75-84 doi.org/10.1016/j.chroma.2016.01.042
Xiao-Li Yin and Hai-Long Wu and Hui-Wen Gu and Yong Hu and Li Wang and Hui Xia and Shou-Xia Xiang and Ru-Qin Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Tartaric acid

Sample.RealLife.Environment
- Wines

Complexity. Sample
- Interferences from other low molecular weight organic acids commonly present in wines

Instrument
- Square wave voltammetry

Process
- Electrocatalytic oxidation on a cobalt(II)-phthalocyanine-modified electrode

Methods.MathStat:
- U-PLS/RBL

Voltammetric determination of tartaric acid in wines by electrocatalytic oxidation on a cobalt(II)-phthalocyanine-modified electrode associated with multiway calibration

Analytica Chimica Acta, 1008(2018)29-37

Anabel S. Lourenço and Raphael F. Nascimento and Amanda C. Silva and Williame F. Ribeiro and Mario C.U. Araujo and Severino C.B. Oliveira and Valberes B. Nascimento

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Nine B-group vitamins

Sample.RealLife.Environment
- Energy drinks
- Complex food matrices

Complexity. Sample
- Co-eluted peaks
- Unknown interferents in LC-MS analysis

Instrument
- LC-MS

Methods.MathStat:
- Alternating trilinear decomposition, ATLD
- Alternating penalty trilinear decomposition, APTLD

Method.Confirmation
- LC-MS/MS

Rapid and interference-free analysis of nine B-group vitamins in energy drinks using trilinear component modeling of liquid chromatography-mass spectrometry data

Talanta, 180(2018)108-119

Yong Hu and Hai-Long Wu and Xiao-Li Yin and Hui-Wen Gu and Rong Xiao and Li-Xia Xie and Zhi Liu and Huan Fang and Li Wang and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Fruit juices

Chem.Syst:
- Azinphos-methyl (AZM)

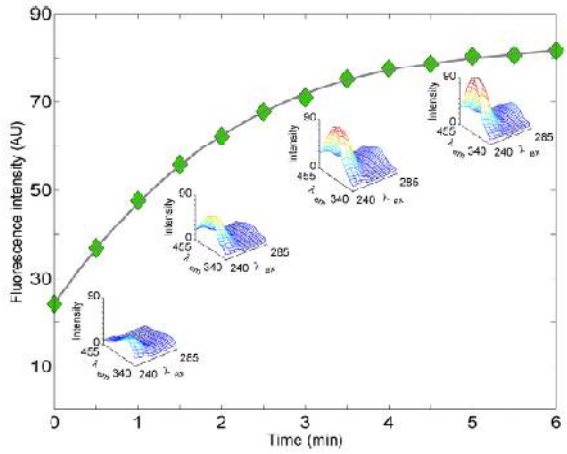
Sample.RealLife.Environment

fruits
- Apple, pear, peach
- Juice samples with and without spiked analyte

Instrument
- Ex.Em.Fl

	Data.Measurement
Step 1	UV-light irradiation of sample
Step 2	EEFSpectra (at 6 min) for five pure standard samples of AZM (in triplicate) & test sample → 3way-(second order) array: [16 (samples) × 21 (excitation wavelengths) × 33 (emission wavelengths)];
Step 3	4way--(Third order) array: (16 × 21 × 33 × 13) thirteen EEFMs recorded; [#Ex x #Em : 21 x 33]; Time#: 13 Number of samples: [15 standards +1 test]

Process	Methods.MathStat:	Order,advantage
o Photochemically induced degradation of AZM into a highly fluorescent product	o PARAFAC o U-PLS/RTL.	Second-order advantage + Un-modelled components Third-order advantage + Improvement in analytical figures of merit



Evolution of EEFintensity as a function of time after irradiation of AZM

Automatic generation of photochemically induced excitation-emission-kinetic four-way data for the highly selective determination of azinphos-methyl in fruit juices	Sensors and Actuators B: Chem, 239(2017)397-404 doi.org/10.1016/j.snb.2016.08.033

Milagros Montemurro and Gabriel G. Siano and María J. Culzoni and Héctor C. Goicoechea

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Highly sensitive quantitation of pesticides in fruit juice samples by modeling four-way data gathered with high-performance liquid chromatography with fluorescence excitation-emission detection	Talanta, 154(2016)208-218 doi.org/10.1016/j.talanta.2016.03.078

Milagros Montemurro and Licarion Pinto and GermanoVéras and Adriano de Araújo Gomes and María J. Culzoni and Mário C. Ugulino de Araújo and Héctor C. Goicoechea

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

PAHs

Chem.Syst:
- 15 PAHs

Sample.RealLife.Environment
- Flue-dust and greasy-dirt samples

Task.Chem.
- Management of urban air quality

Instrument
- GPC-DAD
- Gel permeation chromatography

Complexity. Sample
- Severely overlapped chromatograph peaks
- Highly overlapped chromatograms
- Presence of unexpected interferents

Methods.MathStat:
- ATLD

Alternating trilinear decomposition of highly overlapped chromatograms for simultaneously targeted quantification of 15 PAHs in samples of pollution source

Microchemical Journal, 146(2019)742-752
doi.org/10.1016/j.microc.2019.01.071

Xiang-Dong Qing and Huai-Bo Zhou and Xiao-Hua Zhang and Hai-Long Wu and Chang-Ya Chen and Su-Wen Xu and Shuang-Shuang Li

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- PAHs

Sample.RealLife.Environment
- Tap water
- Hookah water

Task.Chem.
- Resolution
- Identification
- Quantification

Methods.MathStat:
- MCR-ALS

Chemometric-based determination of polycyclic aromatic hydrocarbons in aqueous samples using ultrasound-assisted emulsification microextraction combined to gas chromatography–mass spectrometry

J. Chromatography A, 1413(2015)117-126
doi.org/10.1016/j.chroma.2015.08.026

Mohammad Ahmadvand and Hassan Sereshti and HadiParastar

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

3. Environmetrics

Chem.Syst:
- Fluoroquinolone antibiotics

Sample.RealLife.Environment
- Tap water

Task.Chem.
- Chemical rank estimation

Method	Used to
Discrete Fourier transformation	Project the eigenvectors from the singular value decomposition to frequency space
Robust statistical analysis based on iterative t-test.	To eliminate outliers in Fourier coefficients of each eigenvector
ANOVA.	To differentiate meaningful components from noise

+ Second-order advantage was achieved

Chemical rank estimation for second-order calibration by discrete Fourier transform coupled with robust statistical analysis

Chemometrics and Intelligent Laboratory Systems, 141(2015)47-57
doi.org/10.1016/j.chemolab.2014.12.005

Yong-Jie Yu and Hai-Yan Fu and Hui-Wen Gu and Yong Li and Chao Kang and Yi-Peng Wang and Hai-Long Wu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Ethiofencarb +
- Interferences

Sample.RealLife.Environment
- Tap water.

Data.Measurement
Third variable
- Hydrolysis time

Complexity. Sample
Interferences
- Fenobucarb
- Bendiocarb

Instrument
- Differential pulsed voltammetry

Methods.MathStat:
- MCR-ALS
- U-PLS/RBL

Second-order advantage maintenance with voltammetric data modeling for quantitation of ethiofencarb in the presence of interferences

Talanta, 132(2015)851-856
doi.org/10.1016/j.talanta.2014.10.006

Nielene Mora Diez and Agustina GuiberteauCabanillas and Antonio Silva Rodríguez and Héctor C. Goicoechea

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Pharmaceutical contaminants
- Mazepine
- ofloxacin
- piroxicam

Sample.RealLife.Environment
- Water samples

Task.Chem.
- ExEMFl

Complexity. Sample

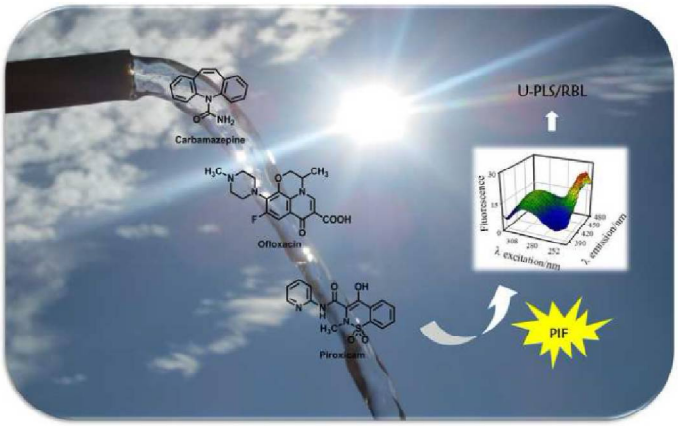
- Interferent media

Complexity. Response data

- Strong spectral overlapping

Method. Chemometric

- After UV irradiation
- Second-order algorithms



Green analytical determination of emerging pollutants in environmental waters using excitation–emission photoinduced fluorescence data and multivariate calibration

Talanta, 134(2015)215-223
doi.org/10.1016/j.talanta.2014.11.022

María del Carmen Hurtado-Sánchez and Valeria A. Lozano and María Isabel Rodríguez-Cáceres and Isabel Durán-Merás and Graciela M. Escandar

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

$$$

Chem.Syst:

Pesticides in the farming industry

- Imidacloprid
- Neonicotinoid

Sample.RealLife.Environment

- Water samples

Methods.MathStat:

- PARAFAC
- U-PLS/RBL

Order advantage.second

Determination of imidacloprid in presence of

- Potential interferences in photo-induced fluorescence
- Other pesticides and/or unexpected compounds

Determination of imidacloprid in water samples via photochemically induced fluorescence and second-order multivariate calibration

Talanta, 134(2015)8-15
doi.org/10.1016/j.talanta.2014.11.017

Edwar Fuentes and Camila Cid and María E. Báez

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- Ciprofloxacin
- Norfloxacin as interferent

Sample.RealLife.Environment

- Water samples

Task.Chem.

- Quantitation

Instrument
- Total synchronous fluorescence spectroscopy

Complexity. Data. Response
- Nonbilinear profile

Methods.MathStat:
- Unfolded partial least squares with residual bilinearization (U-PLS/RBL)

- Extremely large number of RBL factors needed

Remedy : U-PLS/IMNB/MCR-ALS

Methods.MathStat:

(U-PLS/IMNB/MCR-ALS)
- Unfolded partial least squares +
- Interference modeling of non bilinear data by
  - Multivariate curve resolution by alternating least squares

\+ [U-PLS/IMNB/MCR-ALS] >> PARAFAC, U-PLS/RBL MCR-ALS

Modeling nonbilinear total synchronous fluorescence data matrices with a novel adapted partial least squares method

Analytica Chimica Acta, 859(2015)20-28 doi.org/10.1016/j.aca.2014.12.014

Agustina V. Schenone and Adriano de Araújo Gomes and María J. Culzoni and Andrés D. Campiglia and Mário Cesar Ugulino de Araújo and Héctor C. Goicoechea

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Tributyltin

Sample.RealLife.Environment

Environmental samples
- Waters
- Sediments

Task.Chem.
- Multivariate calibration

Instrument
- Ex.Em.Fl

Methods.MathStat:
- U-PLS/RBL

A novel application of nylon membranes for tributyltin determination in complex environmental samples by fluorescence spectroscopy and multivariate calibration

Chemometrics and Intelligent Laboratory Systems, 148(2015)77-84doi.org/10.1016/j.chemolab.2015.09.005

Manuel A. Bravo and Graciela M. Escandar and Alejandro C. Olivieri and Emmanuelle Bardin and Luis F. Aguilar and Waldo Quiroz

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Natural and synthetic sex hormones
- Estrogens,
- Three progestagens
- One androgen
- +
- Real interferences.

Sample.RealLife.Environment
- Environmental waters
- Sediments

Instrument
- LC-[dual UV + Fl]

Methods.MathStat:
- MCR-ALS

Chromatography	Total or partial resolution of a large number of compounds
Dual detection	Selection of the most appropriate signal for each analyte
Second-order calibration	Mathematical resolution of incompletely resolved chromatographic bands Analyte determination in the presence of interferents

Multivariate calibration-assisted high-performance liquid chromatography with dual UV and fluorimetric detection for the analysis of natural and synthetic sex hormones in environmental waters and sediments

Environmental Pollution, 209(2016)114-122 doi.org/10.1016/j.envpol.2015.11.024

Rocío L. Pérez and Graciela M. Escandar

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Waste Water

Chem.Syst:

Six antibiotics
- Amoxicillin
- Metronidazole
- Sulfamethoxazole
- Ofloxacine
- Sulfadiazine
- Sulfamerazine

Sample.RealLife.Environment
- Waste-water samples

Instrument
- HPLC–DAD

Methods.MathStat:
- MCR/ALS and U-PLS/RBL,

Direct analysis of six antibiotics in wastewater samples using rapid high-performance liquid chromatography coupled with diode array detector: A chemometric study towards green analytical chemistry

Talanta, 135(2015)7-17 doi.org/10.1016/j.talanta.2014.12.036

Maryam Vosough and Masoumeh Rashvand and Hadi M. Esfahani and Kazem Kargosha and Amir Salemi

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- PAHs

Sample.RealLife.Environment
- Oil-field wastewaters

Instrument
- Ex.Em.Fl.

Methods.MathStat:
- PARAFAC

Method. Confirmation
- GC–MS method

A green chemometrics-assisted fluorimetric detection method for the direct and simultaneous determination of six polycyclic aromatic hydrocarbons in oil-field wastewaters

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 200 (2018)93-101doi.org/10.1016/j.saa.2018.04.014

Hui-Wen Gu and Shan-Hui Zhang and Bai-Chun Wu and Wu Chen and Jing-Bo Wang and Yang Liu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Seven nitroaromatic compounds

Sample.RealLife.Environment
- Environmental water

Complexity. Sample
- Significantly overlapping peaks

Instrument
- HPLC-DAD

Methods.MathStat:
MCR-ALS

Chemometrics-enhanced high performance liquid chromatography strategy for simultaneous determination on seven nitroaromatic compounds in environmental water

Chemometrics and Intelligent Laboratory Systems, 174(2018) 149-155
doi.org/10.1016/j.chemolab.2017.10.022

Yihuan Zhao and Yuan Yuan and Jianfang Chen and Menglong Li and Xuemei Pu

Marine sediments

Chem.Syst:
- Tributyltin (TBT)

Sample.RealLife.Environment
- Marine sediments

Task.Chem.
- Detection

Instrument
- Ex.Em.Fl

Chem Separation Method
Cloud point extraction (CPE)

Complexity. Sample
- Interferences

Methods.MathStat:
MCR–ALS

Order.advantages

Instrument. second-order. advantage
+ Presence of uncalibrated interferences, E. butyltin compounds or metallic species commonly found in sediment sample extracts

Evaluation of cloud point extraction coupled with fluorescence spectroscopy and multivariate curve resolution–alternating least squares for tributyltin determination in sediment samples

Microchemical Journal, 124(2016)132-138
doi.org/10.1016/j.microc.2015.08.012

Francis Alarcón and Roxana Bustamante and Waldo Quiroz and Luis F. Aguilar and Manuel A. Bravo

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

4. MethodoMetrics

Chemical Rank

Method. Rank.chemical- 3waydata

- Angle distribution of loading subspace (ADLS)

Data.Sets with "non-trilinear" structure

- Simulated
- Real data sets

Complexity. Sample

- \- Noise
- \- Coherence
- \- Low sensitivity component (s)

Inference. ADLS

- \+ ADLS more robust than CORCONDIA
- \+ Results clearer than those based PARAFAC

ADLS based on SWATLD

Three-way analysis

- \+ Unique decomposition of trilinear model
- \+ Clear physical/chemical interpretation
- \+ Second-order advantage
  - \+ Possible quantification of components of interest in complex system with unknown interferents.
- \+ The estimation of chemical rank is a crucial step in three-way analysis.

Methods. chemical rank

Core consistency diagnostic (CORCONDIA):

Based on two three-way analysis algorithms

i.e. parallel factor analysis (PARAFAC)

self-weighted alternating trilinear decomposition (SWATLD)

Angle distribution of loading subspaces (ADLS) for chemical rank estimation in three-way analysis	Chemometrics and Intelligent Laboratory Systems, 152(2016)146-156 doi.org/10.1016/j.chemolab.2015.11.006
Y.J. Liu and J. Jansen and G. Postma and T. Tran and H.L. Wu and L.M.C. Buydens	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

A comparison of several trilinear second-order calibration algorithms	Chemom. Intell. Lab. Syst., 106 (2011) 93-107
Y.J. Yu, H.L. Wu, J.F. Nie, S.R. Zhang, S.F. Li, Y.N. Li, S.H. Zhu, R.Q. Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Models for 3-way data

Chem.Syst:

- Phenanthrene
- Anthracene

Instrument

- GC-MS

Task.Chem.

Second-order calibration algorithms

Effect of noise and shift on multivariate figures of merit

Complexity. Chromatograms	Methods.MathStat:	Figures of Merit
o Noise and peak shifts	▶ MCR-ALS ▶ PARAFAC ▶ PARAFAC2	o Sensitivity (SEN) o Analytical sensitivity (γ) o Selectivity (SEL) o Limit of detection (LOD).
Complexity. Analytes		
o Different two- and three-component systems with interferences Simulated Datasets		

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Data Sets.3way	Weighted alternating penalty trilinear decomposition (W-APTLD)
o One simulation o Two real data sets + o missing values	o Based on the weighted trilinear model Positive features + Deals with missing values + Retains second-order advantage + Overcomes problem due to severe collinearity + Extendable to higher-way data arrays (containing missing values) + Even with excessive factors, it gives more accurate results
Complexity.Data .Multi-way	
o Various malfunctions of instruments o Responses being outside instrument ranges o Irregular measurement intervals between samples and data postprocessing	

Dealing with three-way data containing missing values by new weighted method for second-order calibration	Chemometrics and Intelligent Laboratory Systems, 171(2017)207-217 doi.org/10.1016/j.chemolab.2017.10.021
Yong Li and Hai-long Wu and Xiang-yang Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Task.Visual display.3wayData	DataSets
▶ Canonical variate analysis biplot	o Simulated data o Blue crabs dataset [Gemperline et al.]

Combining simultaneous diagonalisation and methods of the two-way CVA biplot methodology
→ explicitly incorporates the grouped structure of the data.
+ Interpretable in the spirit of the two-way CVA biplot

Visualising grouped three-way data: A common canonical variate analysis biplot	Chemometrics and Intelligent Laboratory Systems,167(2017)232-237 doi.org/10.1016/j.chemolab.2017.06.003
Darryn Williams and Sugnet Gardner-Lubbe	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Three skewed matrix variate distributions	Statistics & Probability Letters, 145(2019)103-109 doi.org/10.1016/j.spl.2018.08.012
Michael P.B. Gallaugher and Paul D. McNicholas	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Three skewed matrix variate distributions	Statistics & Probability Letters, 145(2019)103-109 doi.org/10.1016/j.spl.2018.08.012
Michael P.B. Gallaugher and Paul D. McNicholas	

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Figure of Merit (FoM)

A systematic study on the effect of noise and shift on multivariate figures of merit of second-order calibration algorithms	Analytica Chimica Acta, 952(2017)18-31 doi.org/10.1016/j.aca.2016.11.070
Mohammad Ahmadvand and HadiParastar and Hassan Sereshti and Alejandro Olivieri and Roma Tauler	
3way-068	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Miscellaneous

Chem.Syst:
- o Bisphenol A (BPA)
- o Diphenyl carbonate (DPC)

Sample.RealLife.Environment
- ! Polycarbonate plastics

Instrument
- o [Ex. Em-Fl]

Complexity. Sample
- o Unknown interferences

Complexity. Response.Instrum
- o Spectral overlap
- o Background

Order. Advantages

Instrum.second-order. advantage
- + Precise quantification of two target analytes
- + Presence of severe spectral overlap
- + Unknown and background interferences

Simultaneous and fast determination of bisphenol A and diphenyl carbonate in polycarbonate plastics by using excitation-emission matrix fluorescence couples with second-order calibration method	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 216(2019)283-289 doi.org/10.1016/j.saa.2019.03.039
Yue Chen and Hai-Long Wu and Xiao-Dong Sun and Tong Wang and Huan Fang and Yue-Yue Chang and Li Cheng and Yu-Jie Ding and Ru-Qin Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Intracellular metabolic coenzymes
- o FAD
- o FMN

Sample.RealLife.Environment
- ▪ Cancer cell

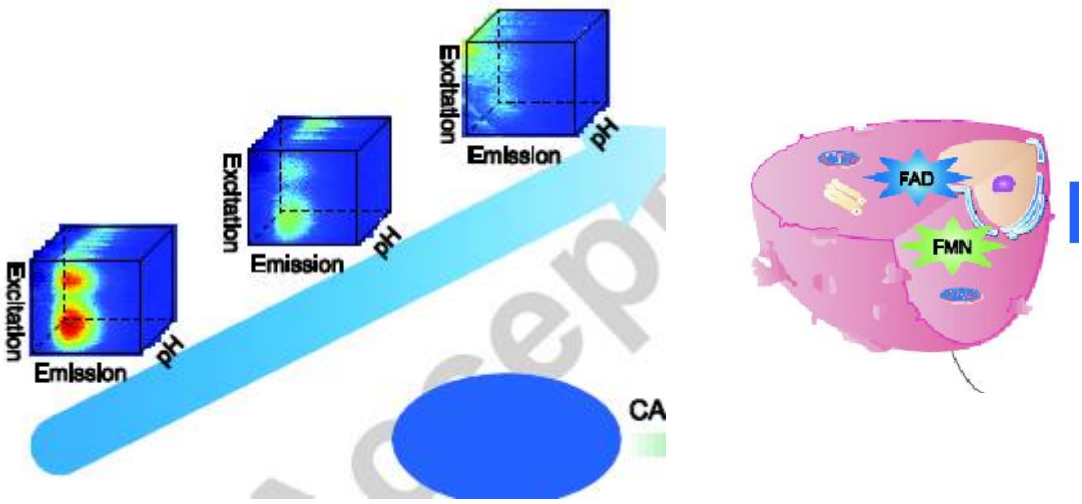
Instrument
- o Ex.Em.Fl

Complexity. Data.Instum.Chromat

- Multiple uncalibrated spectral interferents

Complexity. Mathematical

- High collinearity of data
  → Consequence: trilinear decomposition of three-way calibration data not capable to decompose into pure spectra of FAD and FMN (because of two-factor degeneracies in their trilinear decomposition)
- o Way-Out: four-way calibration



Instrument	Dimension-one	excitation wavelengths	[232-to-500 nm ; Inc: 2 nm]
	Dimension-two	emission wavelengths	[452-to-650 nm ; Inc: 2 nm]
Influencing variable	Dimension-three	Chemical (pH)	[2.2, 2.6, 3.0, 3.4, 3.8, 4.2, 4.6]
Concentration	Dimension-four	Concentration of analyte [#samples]	10

EX-EM-pH-Sample four-way data array : (85 × 100 × 7 × 10)

Calibration Samples

- o Seven samples
- o Expt. Design : U7(72) uniform design for concentrations of FAD and FMN

Third Order.advantage

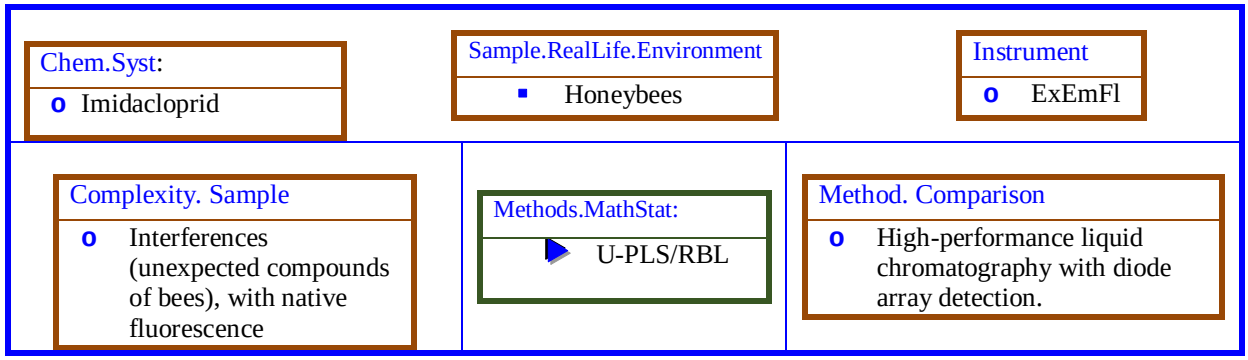
- + Higher sensitivity
- + Enhanced resolving power.

Simultaneously quantifying intracellular FAD and FMN using a novel strategy of intrinsic fluorescence four-way calibration

Talanta, 197(2019)105-112
doi.org/10.1016/j.talanta.2018.12.076

Chao Kang and Hai-Long Wu and Min-Li Xu and Xiu-Fang Yan and Ya-Juan Liu and Ru-Qin Yu

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way



Photochemically induced fluorescence coupled to second-order multivariate calibration as analytical tool for determining imidacloprid in honeybees	Chemometrics and Intelligent Laboratory Systems, 160(2017)1-7 doi.org/10.1016/j.chemolab.2016.11.001
YanaraJeria and AlioshaBazaes and María E. Báez and Jeannette Espinoza and Jessica Martínez and Edwar Fuentes	

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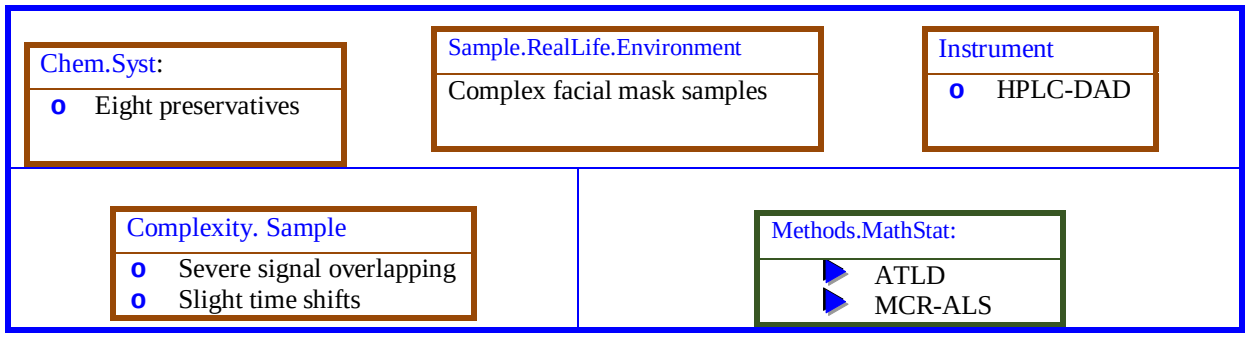
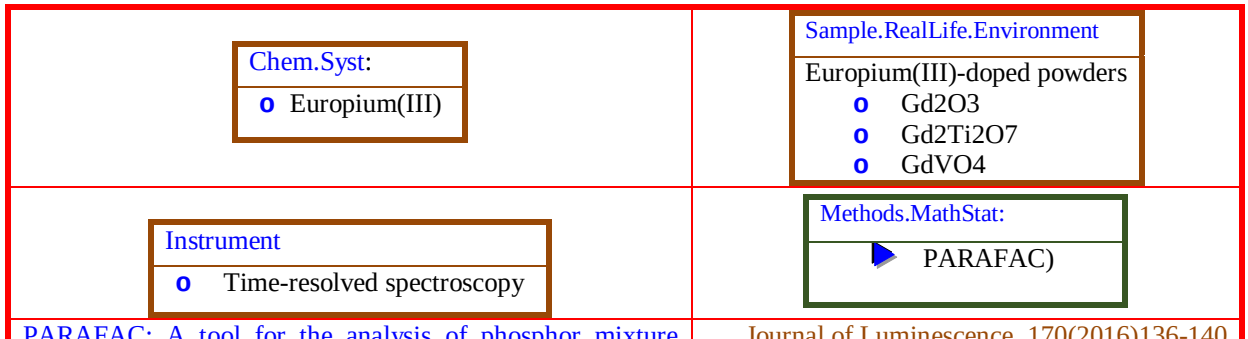


Dealing with overlapped and unaligned chromatographic peaks by second-order multivariate calibration for complex sample analysis: Fast and green quantification of eight selected preservatives in facial masks	Journal of Chromatography A, 1573(2018)18-27 doi.org/10.1016/j.chroma.2018.09.019
Xiao-Li Yin and Hui-Wen Gu and Ali R. Jalalvand and Ya-Juan Liu and Ying Chen and Tian-Qin Peng	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way



PARAFAC: A tool for the analysis of phosphor mixture luminescence	Journal of Luminescence, 170(2016)136-140 doi.org/10.1016/j.jlumin.2015.10.030
Lea Lenhardt and Miroslav D. Dramićanin	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- Ethanol
- Water
- Ethanol–water cluster

Task.Chem.

- Temperature dependence of NIR spectra

Instrument

- NIR

Methods.MathStat:

- Multiway principal component analysis (NPCA),
- Parallel factor analysis (PARAFAC)
- Alternating trilinear decomposition (ATLD)

Chemometric algorithms for analyzing high dimensional temperature dependent near infrared spectra

Chemometrics and Intelligent Laboratory Systems, 170(2017)109-117
doi.org/10.1016/j.chemolab.2017.08.010

Xiaoyu Cui and Jin Zhang and Wensheng Cai and Xueguang Shao

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

- Aniline
- 2,4-diaminotoluene (2,4-tda)
- 4,4′-methylenedianiline (4,4′-MDA)

Method.

- Polyamide cooking utensils

Advantage. Data structure

IfTrilinearity of the data tensor is proved
Then uniqueness of the solution obtained through PARAFAC is guaranteed
➔ **Consequence:** Factors of the decomposition match up with analytes

Migration kinetics of primary aromatic amines from polyamide kitchenware: Easy and fast screening procedure using fluorescence

Talanta, 160(2016)46-55
doi.org/10.1016/j.talanta.2016.06.060

S. Sanllorente and L.A. Sarabia and M.C. Ortiz

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:

Enantiomers

- Lysine (lys),
- Leucine (leu)
- Phenylalanine (phe)

+

- optically active chiral thiol compound, 1-mercapto-2-propanol (MP)

Process

- Amino acid (AA) enantiomers react with each other to yield two fluorescent diasteriomers of D and L-AA with maximum difference in fluorescence intensity at about 450 nm

Methods.MathStat:

- MCR-ALS

Determination of enantiomeric excess of some amino acids by second-order calibration of kinetic-fluorescence data	Analytical Biochemistry, 550(2018)15-26 doi.org/10.1016/j.ab.2018.04.004
AzadehNaghashian-Haghighi and Bahram Hemmateenejad and MojtabaShamsipur	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Nine proteins

Task.Chem.
- Protein secondary structure determination

Instrument
- Multi-excitation ultraviolet resonance Raman spectra

Methods.MathStat:
- PARAFAC

Output
Correlated with the relative abundance of
- Helical
- β-sheet
- Poly-proline II
  - Dihedral angles.

Model
- A three factor model
- Non-negativity constraints
  - ➔ Produced three unique factors

Parallel factor analysis of multi-excitation ultraviolet resonance Raman spectra for protein secondary structure determination	Analytica Chimica Acta, 892(2015)59-68 doi.org/10.1016/j.aca.2015.08.035
Olayinka O. Oshokoya and Renee D. JiJi	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Chem.Syst:
- Irinotecan

Task.Chem.
- Lactone hydrolysis kinetics

Instrument
- EEM

Data.tensor
[EEM] x [inetic] x [Samples]

Methods.mathstat:
- Alternating normalization -weighted error (ANWE)

Complexity. Data

Florescence Spectral profiles
- Fluorescence spectra of CPT-11-L and CPT-11-C seriously overlapped

Analytes
- Unknown fluorescent components in the plasma

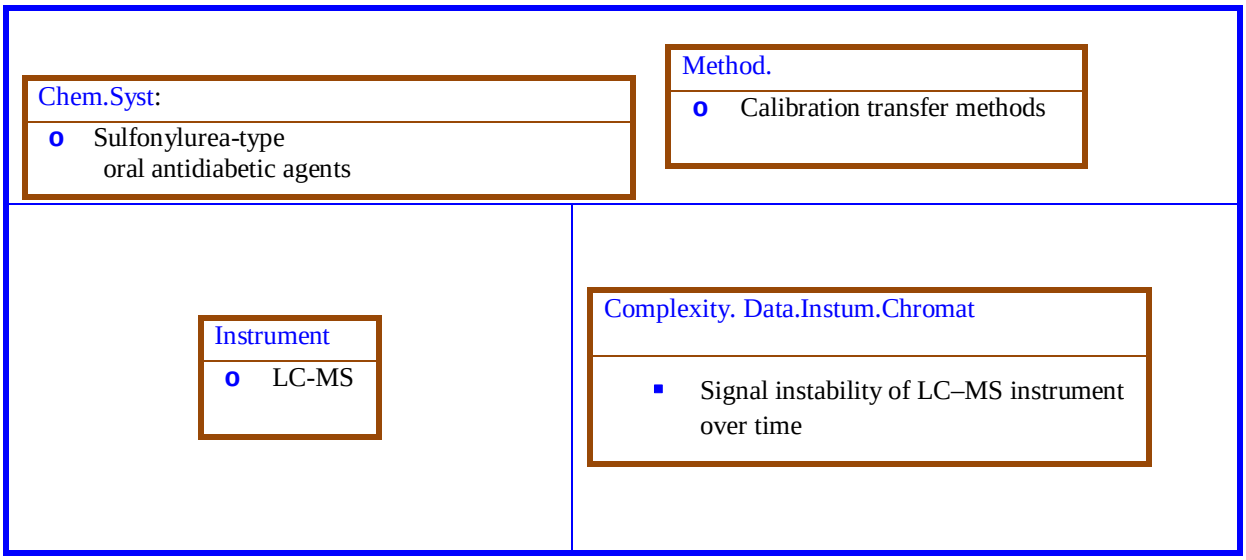
.

Results
- Static samples validation
- Spiked plasma samples
- Kinetic samples

Process.bioChem
- Lactone hydrolysis of irinotecan in human plasma

Second-order calibration method applied to process three-way excitation–emission-kinetic fluorescence data: A novel tool for real-time quantitative analysis of the lactone hydrolysis of irinotecan in human plasma	Chemometrics and Intelligent Laboratory Systems, 146(2015)447-456 doi.org/10.1016/j.chemolab.2015.06.018
Xiao-Li Yin and Hai-Long Wu and Hui-Wen Gu and Yong Hu and Hui Xia and Li Wang and Ru-Qin Yu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way



Solving signal instability to maintain the second-order advantage in the resolution and determination of multi-analytes in complex systems by modeling liquid chromatography–mass spectrometry data using alternating trilinear decomposition method assisted with piecewise direct standardization	Journal of Chromatography A, 1407(2015)157-168 doi.org/10.1016/j.chroma.2015.06.049
Hui-Wen Gu and Hai-Long Wu and Xiao-Li Yin and Shan-Shan Li and Ya-Juan Liu and Hui Xia and Li-Xia Xie and Ru-Qin Yu and Peng-Yuan Yang and Hao-Jie Lu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Current challenges in second-order calibration of hyphenated chromatographic data for analysis of highly complex samples	Journal of Chemometrics, (2017) 1-15
Maryam Vosough	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Second order advantage obtained by spectroelectrochemistry along with novel carbon nanotube modified mesh electrode: Application for determination of acetaminophen in Novafen samples	Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 153(2016) 674-680 doi.org/10.1016/j.saa.2015.09.035
Karim Asadpour-Zeynali and S. Maryam Sajjadi and Fatemeh Taherzadeh	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

TTWD-DA: A MATLAB toolbox for discriminant analysis based on trilinearthree-way data	Chemometrics and Intelligent Laboratory Systems 188 (2019) 46–53 doi.org/10.1016/j.chemolab.2019.03.007
Camilo L.M. Morais a,*, Kassio M.G. Lima b, Francis L. Martin a,**	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

CLV3W: A clustering around latent variables approach to detect panel disagreement in three-way conventional sensory profiling data	Food Quality and Preference, 47(2016) 45-53 doi.org/10.1016/j.foodqual.2015.03.013
Tom F. Wilderjans and VéroniqueCariou	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Investigation of kinetics and thermodynamics of DNA hybridization by means of 2-D fluorescence spectroscopy and soft/hard modeling techniques	Analytica Chimica Acta, 906(2016)58-71 doi.org/10.1016/j.aca.2015.11.039
Sara Ebrahimi and Mohsen Kompany-Zareh	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Wide-range CTAT and PTAT sensors with second-order calibration for on-chip thermal monitoring	Microelectronics Journal, 46(2015)819 - 824
Chua-Chin Wang and Wen-Je Lu and Tzu-Chao Wu	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Connected Categorical Canonical Covariance Analysis for Three-mode Three-way data Sets Based on Tucker Model	Procedia Computer Science, 96(2016)912-319 doi.org/10.1016/j.procs.2016.08.270
Jun Tsuchida and Hiroshi Yadohisa	

3way--3way--3way--3way--3way--3way--3way--3way--3way--3way

Nonlinear fault detection of batch processes based on functional kernel locality preserving projections	Chemometrics and Intelligent Laboratory Systems, 183(2018)79-89 doi.org/10.1016/j.chemolab.2018.10.010
Fei He and Chaojun Wang and Shu-Kai S. Fan	

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Four-way calibration applied to the processing of pH-modulated fluorescence excitation-emission matrices. Analysis of fluoroquinolones in the presence of significant spectral overlapping	Microchemical Journal, 132(2017)211-218doi.org/10.1016/j.microc.2017.01.028
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