

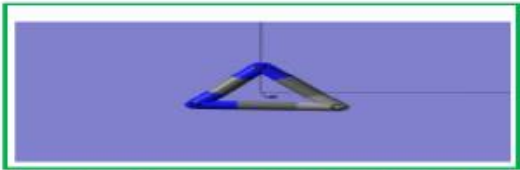
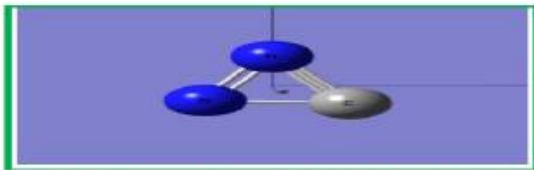


Journal of Applicable Chemistry

2019, 8 (4): 2025-2032
(International Peer Reviewed Journal)



New Chemistry News
 $\text{N}=\text{C}=\text{N}$

 New News of Chem (NNC)	 ChemNewsNew (CNN)
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5-way, 6-way data analysis	Information Source (is) ACS.org Sciencedirect.com
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Pesticides

Chem.Syst: ○ Pesticide	Sample.RealLife.Environment ▪ Artificial river samples spiked with imidacloprid
Instrument ○ Ex.Em.-Fl	Data.5way [Excitation; UV irradiation time; volume] x Samples

Complexity. Data.Instum.Chromat ▪ Matrix effect from environmental water induces partial fluorescence quenching

<p>Process</p> <ul style="list-style-type: none"> ○ Photochemical derivatization <p>Computations</p> <ul style="list-style-type: none"> ○ Higher-order calibration. 	<p>Methods.MathStat:</p> <ul style="list-style-type: none"> ▶ Alternating fitting weighted residue quadrilinear decomposition (AFWRQLD)
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<p>High-order calibration for the spectrofluorimetric determination of pesticides based on photochemical derivatization. A solution of the problems of inner-filter effects and matrix interferences in complex environmental water</p>	<p>Chemometrics and Intelligent Laboratory Systems 156 (2016) 36–53 doi.org/10.1016/j.chemolab.2016.05.004</p>
<p>Jin-Fang Nie and Bo Li and Yun Zhang and Jin-Long Fan and Zhong-Sheng Yi and Zhi-Rong Cai</p>	

<p>Chem.Syst:</p> <p>Pesticide</p> <ul style="list-style-type: none"> ○ Carbaryl <p>Interferents -- fungicides</p> <ul style="list-style-type: none"> ○ Fuberidazole ○ Thiabendazole <p>Interferents uncalibrated</p>	<p>Process</p> <ul style="list-style-type: none"> ○ Hydrolysis of fluorescent analyte ○ Fluorescence excitation-emission- data. Specifically, <ul style="list-style-type: none"> ➔ produce 1-naphthol which also emit fluorescence
<p>Instrument</p> <ul style="list-style-type: none"> ○ ExEmFlfast-scanning <p>Influence.variables</p> <ul style="list-style-type: none"> ○ Kinetic time ○ pH 	<p>Data.Tensor</p> <ul style="list-style-type: none"> 📖 Fourth Order 📖 Five way ❓ Quadrilinear
<p>Complexity. Data.Instum.Chromat</p> <ul style="list-style-type: none"> - Lack of quadrilinearity of experimental data. 	<p>Methods.MathStat:</p> <p>Latent structured algorithms</p> <ul style="list-style-type: none"> ▶ U-PLS with residual quadri-linearization ▶ PARAFAC

<p>Unfolded partial least-squares with residual quadrilinearization: A new multivariate algorithm for processing five-way data achieving the second-order advantage. Application to fourth-order excitation-emission-kinetic-pH fluorescence analytical data</p>	<p>Chemometrics and Intelligent Laboratory Systems 109 (2011) 178–185 doi.org/10.1016/j.chemolab.2011.09.002",</p>
<p>Rubén M. Maggio a, Arsenio Muñoz de la Peña b, Alejandro C. Olivieri</p>	

<p>Chem.Syst:</p> <ul style="list-style-type: none"> ○ Diclofenac sodium 	<p>Sample.RealLife.Environment</p> <ul style="list-style-type: none"> ▪ Environmental water 	<p>Task.Chem.</p> <ul style="list-style-type: none"> ○ Detection of pharmaceutical pollutants
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<p>Complexity. Response.FI</p> <p>Fluorescence properties of the analyte highly dependent on</p> <ul style="list-style-type: none"> ○ pH ○ Irradiation time in situ 	<p>Data.Measurement Per sample</p> <ol style="list-style-type: none"> 1) Emission 2) Excitation 3) Time- 4) pH
<p>Figures of Merit.</p> <ul style="list-style-type: none"> ○ Statistical analysis <ul style="list-style-type: none"> ○ Elliptical joint confidence region test ○ t-test 	<p>Methods.MathStat:</p> <ul style="list-style-type: none"> ▶ Alternating fitting weighted residue quinquelinear decomposition (AFWRQQLD), ▶ Five-way parallel factor analysis (five-PARAFAC) ▶ Alternating quinquelinear decomposition (AQQLD).

<p>Fluorescent kinetics combined with fourth-order calibration for the determination of diclofenac sodium in environmental water</p>	<p>Analytical and Bioanalytical Chemistry, 2019, 411(10), 2019–2029 https://doi.org/10.1007/s00216-019-01624-5</p>
<p>Jiao Li & Jie Xu & Wenying Jin & Zhongsheng Yi & Chenbo Cai & Xuefen Huang & Jinfang Nie & Yun Zhang</p> <p>5way--5way--5way--5way--5way--5way--5way--5way--5way--5way--5way--</p>	

Herbicides

<p>Chem.Syst:</p> <ul style="list-style-type: none"> ○ Naptalam (NAP) ○ Interferen <ul style="list-style-type: none"> ○ IAA ○ NAD 	<p>Instrument</p> <ul style="list-style-type: none"> ○ HPLC-DAD <p>Influence.variables</p> <ul style="list-style-type: none"> ○ Kinetic time ○ pH 	<p>Data.5way</p> <ol style="list-style-type: none"> 1) [Retention time x 2) Spectra x 3) kinetic time x 4) pH x 5) Samples]
<p>Methods.MathStat:</p> <ul style="list-style-type: none"> ○ Alternating quinquelinear decomposition (AQQLD) ○ Five-way parallel factor analysis (PARAFAC) <p>Basis.AQQLD</p> <p>Pseudo-fully stretched matrix forms of the quinque-linear model</p> <ul style="list-style-type: none"> + Faster convergence + Insensitive to the excess number of components 		

<table border="1"> <tr> <td>Method. Chemometric</td> <td></td> </tr> <tr> <td>NAP</td> <td>4 calibration solutions</td> </tr> <tr> <td>Degradation reaction</td> <td>pH: [1.5,1.7, 1.9]</td> </tr> </table> <table border="1"> <tr> <td>[[Instruments]; (Variables)]</td> <td>[Output]</td> </tr> <tr> <td>{HPLC–DAD–}</td> <td>Retention Time_ Wavelength_</td> </tr> <tr> <td>(kinetic–pH)</td> <td>Reaction time_ pH</td> </tr> <tr> <td>Data tensor</td> <td>dimensions 291_76_6_3</td> </tr> </table>	Method. Chemometric		NAP	4 calibration solutions	Degradation reaction	pH: [1.5,1.7, 1.9]	[[Instruments]; (Variables)]	[Output]	{HPLC–DAD–}	Retention Time_ Wavelength_	(kinetic–pH)	Reaction time_ pH	Data tensor	dimensions 291_76_6_3	<table border="1"> <tr> <td>Data. Simulated</td> <td></td> </tr> <tr> <td>Samples</td> <td>16</td> </tr> <tr> <td>Species</td> <td>Three</td> </tr> <tr> <td>Dimensions</td> <td>40_35_30_11_16</td> </tr> </table>	Data. Simulated		Samples	16	Species	Three	Dimensions	40_35_30_11_16
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Dimensions	40_35_30_11_16																						
<table border="1"> <tr> <td>IAA, NAD and unexpected component(s) as interferents</td> <td>five-way data array with dimensions 291_76_6_3_10</td> </tr> </table>	IAA, NAD and unexpected component(s) as interferents	five-way data array with dimensions 291_76_6_3_10																					
IAA, NAD and unexpected component(s) as interferents	five-way data array with dimensions 291_76_6_3_10																						

A novel fourth-order calibration method based on alternating Quinque-linear decomposition algorithm for processing high performance liquid chromatography–diode array detection–kinetic-pH data of naptalam hydrolysis	Analytica Chimica Acta 861 (2015) 12–24
Xiang-Dong Qing, Hai-Long Wu , Xi-Hua Zhang, Yong Li, Hui-Wen Gu, Ru-Qin Yu	
5way--5way--5way--5way--5way--5way--5way--5way--5way--5way	

Heavy metals

<table border="1"> <tr> <td>5way-004</td> </tr> <tr> <td><i>Chem.Syst:</i></td> </tr> <tr> <td>Heavy metals</td> </tr> <tr> <td> <ul style="list-style-type: none"> ○ Cu, Cd, Zn, Al, ○ Pb, Fe, Mn </td> </tr> </table> <table border="1"> <tr> <td>Sample.RealLife.Environment</td> </tr> <tr> <td> <ul style="list-style-type: none"> ▪ Contaminated soil. </td> </tr> </table>	5way-004	<i>Chem.Syst:</i>	Heavy metals	<ul style="list-style-type: none"> ○ Cu, Cd, Zn, Al, ○ Pb, Fe, Mn 	Sample.RealLife.Environment	<ul style="list-style-type: none"> ▪ Contaminated soil. 	<p>Task.Chem.</p> <ul style="list-style-type: none"> <u>?</u> To evaluate effectiveness of the remediation procedure for soil type <u>?</u> Comparison of changes in mobility of metals ‘before’ and ‘after’ treatment <u>?</u> Estimation of influence of pH on the mobility of metals in amended/non-amended soils <p>Aim of the analysis</p> <ul style="list-style-type: none"> ▶ Influence of the initial pH levels (way 1) on the process of ▶ Immobilization of metals (way 2) supposedly bound in different ▶ Forms (way 3) in soil samples with various organic contents (way 4). ▶ ‘Before’ and ‘after’ treatment of soil(way5)
5way-004							
<i>Chem.Syst:</i>							
Heavy metals							
<ul style="list-style-type: none"> ○ Cu, Cd, Zn, Al, ○ Pb, Fe, Mn 							
Sample.RealLife.Environment							
<ul style="list-style-type: none"> ▪ Contaminated soil. 							

Data.5way

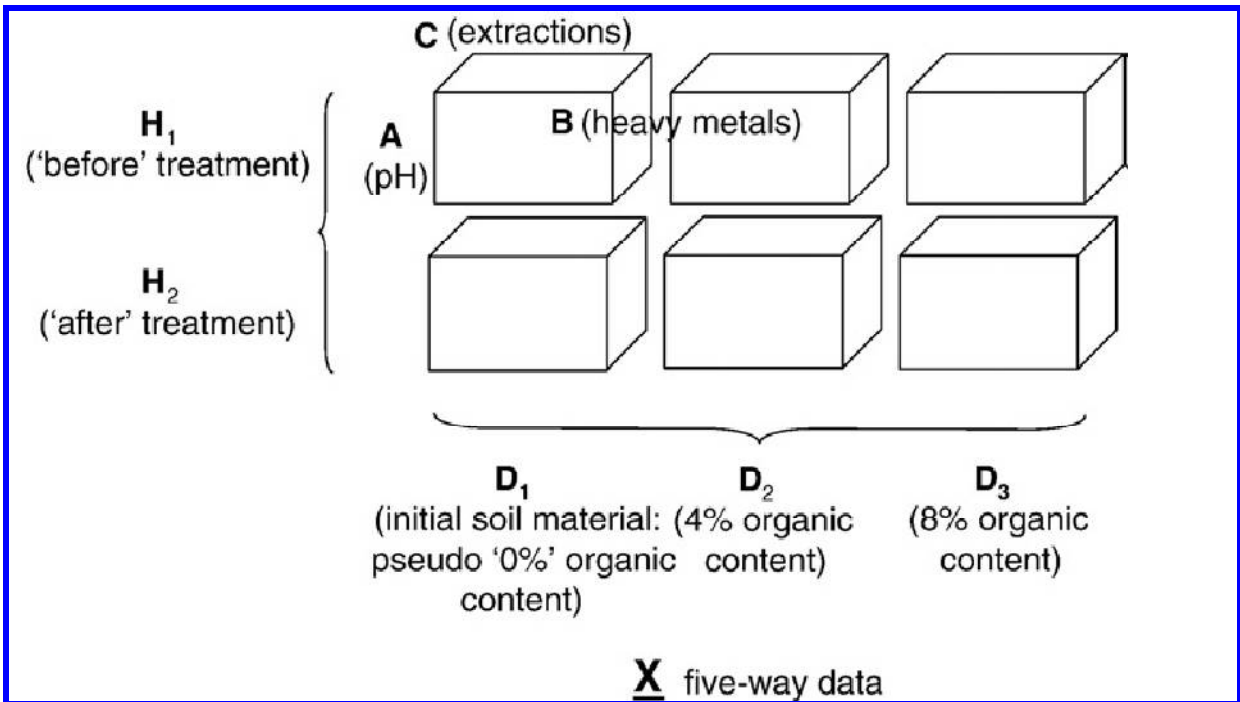
Variables per sample

- 1) pH ×
- 2) Heavy metals extractions ×
- 3) Organic content ×
- 4) Time

Methods.MathStat:

- ▶ Five-mode Tucker model
 - Definite complexity

Output	
→ Influence of soil pH	📖 Way 1
→ Process of immobilization of those heavy metals	📖 Way 2
→ Supposedly bound in different forms	📖 Way 3
→ In heavily contaminated soil samples amended with different amounts of organic matter	📖 Way 4
→ Over time	📖 Way 5



N-way exploration of environmental data obtained from sequential extraction procedure

Chemometrics and Intelligent Laboratory Systems 96 (2009) 203–209

I. Stanimirova a, A. Kita b, E. Malkowski c, E. John a, B. Walczak

5way--5way--5way--5way--5way--5way--5way--5way--5way--5way--5way

Chapter 7 - Unfolded and Multiway Partial Least-Squares with Residual Multilinearization: Fundamentals

editor = "Arsenio Muñoz de la Peña and Héctor C. Goicoechea and Graciela M. Escandar and Alejandro C. Olivieri",
 series = "Data Handling in Science and Technology",
 publisher = "Elsevier",
 29,2015,347 - 363
doi.org/10.1016/B978-0-444-63527-3.00007-2

"Alejandro C. Olivieri and Graciela M. Escandar and Héctor C. Goicoechea and Arsenio Muñoz de la Peña

5way--5way--5way--5way--5way--5way--5way--5way--5way--5way

Chapter 8 - Unfolded and Multiway Partial Least-Squares with Residual Multilinearization: Applications

Data Handling in Science and Technology
 Elsevier, 29(2015)365-397
doi.org/10.1016/B978-0-444-63527-3.00008-4

Alejandro C. Olivieri and Graciela M. Escandar and Héctor C. Goicoechea and Arsenio Muñoz de la Peña

5way--5way--5way--5way--5way--5way--5way--5way--5way--5way

Analytical chemistry assisted by multi-way calibration: A contribution to green chemistry

204,2019, 700-712
<https://doi.org/10.1016/j.talanta.2019.06.022>

Alejandro C. Olivieri and Graciela M. Escandar

5way--5way--5way--5way--5way--5way--5way--5way--5way--5way

6way--6way--6way--6way--6way--6way--6way--6way--6way--6way--

Chem.Syst:

- o Drug (antidepressant)

Task.Chem.

Testing phase of a new drug
 ! Appropriate model for effect on activity of brain

Instrument

- o Electroencephalograph (EEG)

#Dimensions	#components
o Subject	o Three
o Spatial	o Three
o Dose	o Two
o Time	o Two
o Condition	o One

Methods-To Explore 6way data→

Multi-way methods	
o Unfolding PCA	Tucker 1
o PARAFAC	Two components
o Tucker	3 model
Six-way	222222.

Data.6way

Data.Structure

Multidimensional structure
 Multi-way modelsused

Six-way array dimensions :

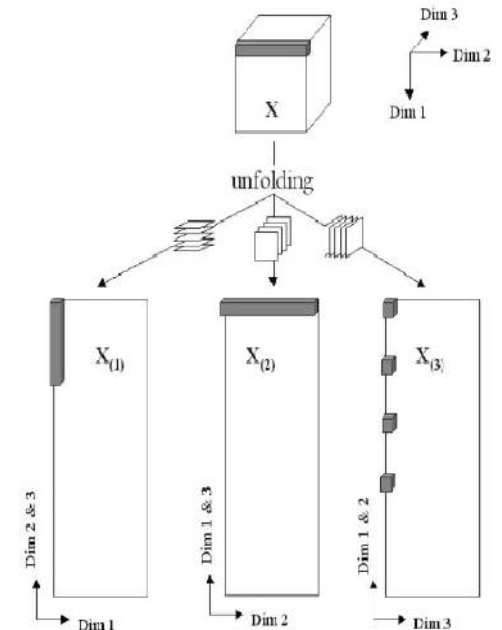
7 x 12 x 28 x 4 x 12 x 2

Complexity. research

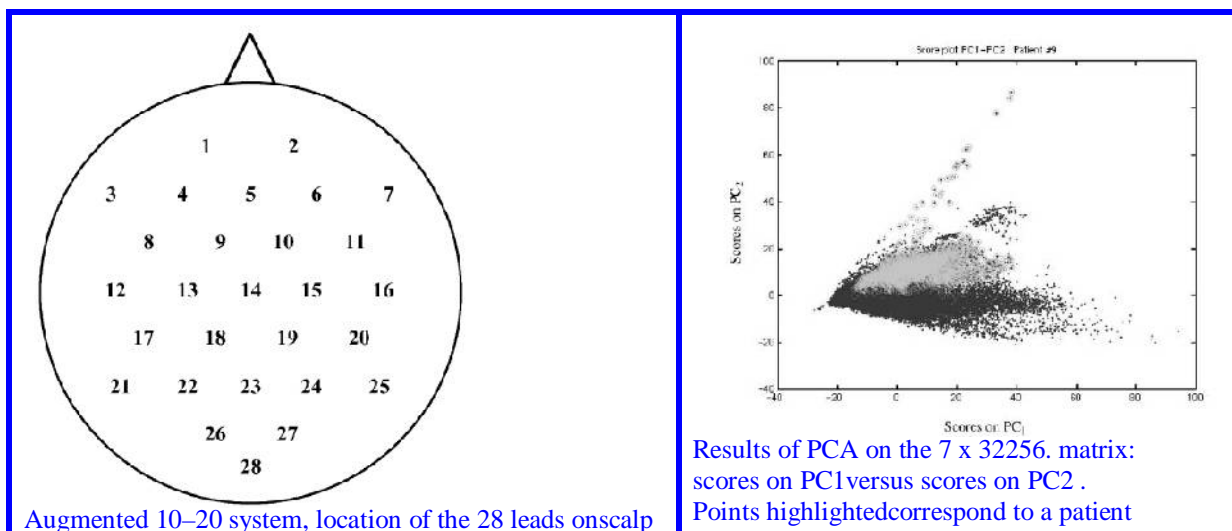
Initial111111.
 Final 333333..
 optimal 333221.,
 o EEG dimension Three components

Phase II trial of antidepressant drug along with placebo

○ Subjects	✓ 12 healthy males
○ Effect of placebo	✓ Four doses ✓ [10, 30 ; 90] mg
○ Time	2-day period ✓ First day : [8:00, 8:30, 9:30, 10:00, 10:30, 11:00, 11:30, 12:00 AM, 1:00 ; 3:00 PM] ✓ Second day: [9 AM; 9 PM] ✓ Total: 12 measurements
○ EEGs	✓ 28 leads augmented 10–20 system repeated twice Seven EEG bands ($\alpha_1, \alpha_2, \beta_1, \beta_2, \beta_3, \delta, \theta$)
○ Dose dimension	■ Four doses: [placebo, 10,30 and 90 mg drug]
○ First measurement	✓ Resting condition i.e. patient lying with eyes closed in a silent room
○ Second measurement	✓ Vigilance-controlled condition, i.e. subject is asked to perform simple tasks while the EEGs are acquired
○ Overall measurements	✓ 32256
○ Software	✓ N-way Toolbox



Unfolding a three-way array X . $X_{(1)}$; $X_{(2)}$; $X_{(3)}$: two-way matrices after unfolding preserving 1st, 2nd and 3rd modes respectively



Multi-way modelling of high-dimensionality
electroencephalographic data

Chemometrics and Intelligent Laboratory
Systems 58 2001. 59–72

F. Estienne , N. Matthijs , D.L. Massart, P. Ricoux, D. Leibovici

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ACS.org ; sciencedirect.com : Information Source

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