



UNIVERSITÄT LEIPZIG

Research Academy Leipzig

SCIENTIFIC AND METHOD MODULES

Module name	Chemometrics applied to spectroscopic data	
Number	2019-B6	
Aims	 To develop an understanding of the application of chemometrics to spectroscopic data analysis To gain a basic overview of how to process spectral data for multivariate analysis Learn how to apply Principal Component Analysis, Partial Least Squares Discriminant Analysis and Partial Least Squares Regression to spectroscopic data using <i>The Unscrambler</i> 	
Contents	 Understand that the Universe is multivariate and applications of multivariate statistics Explore types of data used in chemometrics Near-IR, Raman and IR, qualitative Distinguish between classification (PCA) and regression modelling Explain the difference between objects, variables including continuous and discrete variables Describe ordinal, binary and category, dummy variables Input data into Unscrambler Plot line plots, bar plots, matrix plots Identify noise and variance in spectra Explain "Explained Variance" Define PCs, scores, loadings, residuals, variance and the PCA model equation Know the pre-processing approaches for spectral data (baseline correction, derivatives, reduce average, mean centring, smoothing, normalisation, standard normal variate, Multiplicative scatter correction) Be able to detect outliers Partial Least Squares Regression Analysis 	
Туре	Two-day block course	

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Date (month/year)	October 15 (12 – 6 pm), October 16 (8 – 10 am & 12:30 – 6:30 pm)	
	2019	
Time	see schedule next page	
Location	PC-Pool TA (Room 425/426, Technikum/Analytikum; Linnéstr. 3,	
	04103 Leipzig)	
Work load	15 hours presence/ 45 hours self-study	
Examination	Written exam with multiple choice questions on October 16th 2019	
Credit points	2	
Responsible scientists	Bayden Wood, Philip Heraud, Monash, Australia	
Guest lecturers	Bayden Wood, Philip Heraud, Monash, Australia	
Industrial partners	None	
Recommendations for	Multivariate Data Analysis 6th Edition, K. H. Esbensen & B.	
literature	Swarbrick, 2018, CAMO Analytics	

PRELIMINARY TIME SCHEDULE

Time	Lecturer	Title		
Tuesday, October 15th 2019, Location: PC-Pool TA				
12:00 Welcome				
12:15	Wood	The World is multivariate		
	Heraud	Introduction to multivariate data analysis (Unscrambler Exercises 1 and 2 data input and plotting spectra)		
15:00 Coffee break				
15:30- 18:00	Wood / Heraud	Spectral pre-processing		
	Wood / Heraud	Principal Component Analysis		
	Wood / Heraud	Exercises 3 and 4 (Preprocessing data and PCA)		
Wednesday, October 16th 2019, PLS-DA and PLS-R, Location: PC-Pool TA				
8:30	Wood / Heraud	Tute on Infrared and Raman spectroscopy		
10:00 Break / Lunch (individually)				
12:30	Wood / Heraud	PLS-DA (Exercise 5-6)		
14:00 Coffee break				
14:30	Wood / Heraud	PLS-R (Exercises 7-8)		
16:30 <i>Coffee break</i>				
16:30-18:30 Scientific discussions on students data; examination				

Status 8.10.2019