Webinar Programme
Chemometrics in Vibrational Spectroscopy
Faculty of Chemistry, Jagiellonian University in Krakow
Raman Imaging Group
13th-14th July 2020

Monday, 13th July 2020

10:00 – 10:05 OPENING: Dr. Katarzyna Majzner

Chairman: Prof. Małgorzata Barańska

10:05 – 11:05	**Prof. Beata Walczak**	UŚ	*Basic rules in data modeling*
11:15 – 12:00	**Prof. Hugh Byrne**	FOCAS, DIT	*Quantitative analysis of biological samples using vibrational spectroscopy – examples of Partial Least Squares Regression*
12:10 – 12:25	**Paulina Kozioł**	IFJ PAN	*Histopathological classification of FT-IR data and model translation to QCL modality using variable selection*

12:30 – 13:00 BREAK

Workshop 1 Chairman: Dr. Anna Borkowska

13:00 – 13:45	**Dr. Claudia Beleites**	Chemometrix	*One-class classifiers*
14:00 – 15:30	**Dr. David Perez-Guaita**	FOCAS	*Extracting biological information from infrared and Raman Spectra*

Tuesday, 14th July 2020

Workshop 2 Chairman: Prof. Kamilla Małek

9:00 – 9:30	**Dr. Tomasz P. Wróbel**	Solaris	*The importance of denoising for obtaining high quality and high throughput spectroscopic IR imaging data*
9:40 – 11:10	**Dr. Alex Henderson**	University of Manchester	*Too good to be true? How to validate your data*

11:20 – 13:00 BREAK

Workshop 3 Chairman: Dr. Habil. Katarzyna Marzec

13:00 – 13:45	**Dr. Claudia Beleites**	Chemometrix	*Tutorial on analyzing spectroscopic data in R/hyperSpec, combined with reproducible data analysis with knitr/rmarkdown*
14:00 – 15:30	**Dr. Artur Surówka**	AGH	*First steps with Orange/Quasar - a new powerful, open-source tool for spectroscopic analysis*

15:45 – 15:50 CLOSING: Dr. Katarzyna Kamińska

Organizers:
Dr. Katarzyna Majzner
Dr. Katarzyna Kamińska

Organizing committee:
Ewa Machalska (secretary, email: zor@chemia.uj.edu.pl)
Ewelina Bik
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