



Webinar Program

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. Malgorzata Barańska

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

12:30 – 13:00 BREAK

Workshop 1 Chairman: Dr. Anna Borkowska

13:00 – 13:45	Dr. Claudia Beleites	Chemometrix	<i>One-class classifiers</i>
14:00 – 14:45	Prof. Bayden Wood/ Callum Gassner	Monash University	<i>FTIR imaging of embryonic tissues using Cytospec</i>

14:55 – 15:10 BREAK

15:10 – 16:15	Dr. David Perez-Guaita	FOCAS	<i>Extracting biological information from infrared and Raman Spectra</i>
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Tuesday, 14th July 2020

Workshop 2 Chairman: Prof. Kamilla Malek

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

11:20 – 13:00 BREAK

Workshop 3 Chairman: Dr. Habil. Katarzyna Marzec

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



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
Karolina Chrabąszcz
Aleksandra Dorosz
Adriana Filipek