**82p2 "Aktion Österreich - Tschechische Republik 2018"**

between the

Palacky University Olomouc (PUO) & the Vienna University of Technology (VUT)

Project: MOVISS Bio&Data

**Final report**

Bio&Data was the second workshop of the newly established MOVISS – “Mountain Village Science Series”. It took place in Vorau (Austria) from September 9-12, 2018. It was a small, problem-driven meeting, full of discussions and questions about how to deal with metabolomic data reasonably. A lot of questions from the field of metabolomics and statistics were discussed. The whole meeting was divided into four sessions, every focused on one specific part of the metabolomic experiments. The first part called “Shiny design: What is important when designing experiments?” was targeted on pitfalls connected with the design of the experiment. In the second session called “Misty mountains: How to find peaks hidden in mists? What is a real peak?” was discussed peak detection and the other parts of the initial metabolomic analysis including preprocessing and data normalization. The third part “Mountain safety: awareness of strengths and weakness of statistical tools” was focused on statistical analysis including univariate and multivariate methods. The topic of log-ratio methodology of compositional data was discussed. The last session “Home run: Results Interpretation – Be creative, critical and think next?” was directed to the interpretation of metabolomics experiments with a demonstration of real data sets. A summary of all discussions is planned to be produced as a paper for publication to share within the wider metabolomic community in the next year.

The workshop had truly international character since 68 participants from the Czech Republic, the Netherlands, Germany, USA, Poland, United Kingdom Austria, Hungary, Italy, Canada, Greece, Singapore, and California. The program of contributions of invited speakers was as follows:

Opening lecture

Age Smilde, Open issues in metabolomics data analysis

1) Morning Session: „Shiny design: What is important when designing experiments?

Steffen Neumann – From profiling to biochemical insights

2) Misty mountains: How to find peaks hidden in mists? What is a real peak?

Tomáš Pluskal – Reaching the summit: the importance of feature detection

3) Mountain safety: awareness of strengths and weakness of statistical tools

Beata Walczak – Again about data pre-processing

Johan Westerhuis - Variable selection and classification in the presence of observation below the detection limit using error rate p-values

4) Home run: Results Interpretation – Be creative, critical and think next?

Royston Goodacre: Mass Appeal: lessons learnt from large-scale mass spectrometry-based metabolomics

The aim of this meeting was to bring together undergraduate students, Ph.D. students and early career postdocs from the field of chemistry, biochemistry, and statistics with prominent experts in the respective fields and to teach the attendees all necessary skills for metabolomic data analysis. This purpose has been fulfilled. Students and postdocs were acquainted with the whole process of the metabolomic experiment from its planning, through processing to evaluation. They realized the complexity and the importance of planning all the processes. They also learned new approaches that they can now apply to their own projects. They improved their statistical knowledge which can help in their future scientific career because these skills are not so common in biochemical sciences, but they become very important. All of the participants engaged extensively in the discussions, so they also practiced communicative skills. In order to strengthen the statistical part of the discussions four PhD students from Technical University Wien: Šárka Brodinová, Irene Hoffmann, Fabian Schroeder, and Jan Walach were included in the project.

The meeting was very successful, discussions were very fruitful, and all participants are interested in its continuation of the MOVISS series. The next meeting is planned to be held in the Czech Republic in 2020. The cooperation of both parts was very rewarding, because both groups are focused on the specific issues connected with chemometrics and metabolomics that can be involved in future cooperation projects. Both Czech and Austrian groups shared the experiences with metabolomic data processing, evaluation, and data interpretation. Statistical methods based on univariate and multivariate approaches were also shown with the application on data from clinical metabolomics.

List of participants supported by project and their contributions:

Research participants from the Czech Republic and their contributions:

• prof. RNDr. Tomáš Adam, Ph.D. - He moderated the discussion in the last session connected with the interpretation of the results from metabolomic project. He also talked about the biological interpretation of metabolomic experiments.

• assoc. prof. RNDr. David Friedecký, Ph.D. - He moderated the discussion in the first session connected with design of experiment of the metabolomic project.

All researchers also participated on contributions of students from the Czech Republic as supervisors.

Student and postdoc participants from the Czech Republic and their contributions:

Mgr. Lukáš Najdekr Ph.D., Mgr. Jitka Široká Ph.D., RNDr. Jaroslava Jáčová, Mgr. Radana Karlíková, Mgr. Štěpán Kouřil, Mgr. Lucie Mádrová, Mgr. Julie Rendlová, Ing. Jan Václavík, Eliška Ivanovová, Mgr. Kateřina Mičová Ph.D.

1. Lucie Mádrová, Matyáš Krijt, Veronika Barešová, Jan Václavík, David Friedecký, Dana Dobešová, Olga Součková, Václava Škopová, Marie Zikánová, Tomáš Adam. Mass spectrometric analysis of purine de novo biosynthesis.
2. Štěpán Kouřil, Julie Rendlová, David Friedecký, Tomáš Adam. Removing false features in metabolomics data using correlations.
3. Jitka Široká, Lucie Mádrová, Radana Karlíková, Štěpán Kouřil, Radek Jorda, Vladimír Kryštof, David Friedecký, Tomáš Adam. Effect of cyclin-dependent kinase 4/6 inhibitors on cellular metabolome regarding selectivity.
4. Jan Václavík, Lucie Mádrová, Radana Karlíková, David Friedecký,Leo AJ Kluijtmans, Ron A Wevers, Tomáš Adam. Acylcarnitine profile of 3-hydroxy-3-methylglutaryl CoA lyase deficiency patients.

Research participant from Austria and his contribution:

• Univ. Prof., Dr. techn., Dipl.-Ing. Peter Filzmoser - He moderated the discussion on the statistical analysis of the metabolomics project. He also participated on contributions of students from Austria as a supervisor.

Student participants from Austria and their contributions:

• Dipl.-Ing. Christopher Rieser - logistic regression for high dimensional data (poster presentation).

• Dipl.-Ing. Fabian Schroeder - Nonparametric test for class separability of filter-type model selection (poster presentation).

Website: http://www.moviss.eu/

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