Contribution ID: **16** Type: **not specified**

Using Advanced Metabolome Annotation Workflow to elucidate Microbial Interactions in Microalgae

Microbial communities reveal complex metabolic interactions which critically influence the ecosystem around them. In this instance, we study the interaction in an aquatic ecosystem between the microalgal species Prymnesium parvum, which produces fish killing toxins, and the diatom Skeletonema marinoi, which causes algal blooms. To decipher the roles of individual microorganisms within their complex community, there is a need to identify the specific metabolites causing the observed effects. Most of these metabolites, however, remain uncharacterized.

To address this issue, we use the untargeted metabolomics approach to investigate known and unknown compounds. The two microalgae are grown in a co-culture chamber, separated by a permeable membrane which allows the exchange of exometabolome. The endo- and exometabolome data are extracted from the co-culture samples and analyzed by comparing them to mono-culture samples, which are taken as control. We present here a MS1 pre-processing workflow as addition to the Metabolome Annotation Workflow (MAW) which takes untargeted LC-MS2 spectra as input data. To feed the data generated from LC-MS2 measurements into MAW, pre-processing on MS1 level is crucial and prepares the data for two major tasks: (1) feature annotation and candidate selection by MAW and (2) statistical analysis to find significant features from the complex mix of metabolites. The MS1 pre-processing workflow includes all essential steps for LC-MS1 data analysis, with prior peak picking parameter optimization. The workflow starts with peak detection and retention time correction and yields feature tables, which are then statistically analyzed by PCA, OPLS-DA, variation partitioning and more. Additionally, the MS2 spectra are reconstructed and linked to their MS1 origin for annotation by MAW.

Unsupervised statistical analysis of the exometabolome showed significant differences between co-culture and mono-culture samples, suggesting a change in excreted metabolomes for the microorganisms grown in the co-culture experiment. Using variable selection we will identify the features and in turn the metabolites underlying this relationship. The results from these metabolomic analyses can later be integrated into a multi-omics approach and combined with transcriptomics data to give an overview of this experimental microbial co-culture.

Primary authors: ABEL, Anne-Susann; ZULFIQAR, Mahnoor (Friedrich-Schiller-Universität Jena)

Co-authors: SYHAPANHA, Kristy Southysa (Friedrich-Schiller-Universität Jena); Prof. POULIN, Remington X.; COSTA WARNAKULASURIYA D., Sassrika Nethmini (Friedrich-Schiller-Universität Jena); POHNERT, Georg Alfons Heiner (Friedrich-Schiller-Universität Jena); STEINBECK, Hans Christoph (Friedrich-Schiller-Universität Jena); Dr PETERS, Kristian; Dr SOROKINA, Maria

Presenter: ABEL, Anne-Susann

Session Classification: Poster session