

Examination of algorithms for deconvolution and library-searching in non-target analysis (Expert Meeting 28th November in Thessaloniki)

Background:

Hypothesis: Data-processing tools and routines differ between laboratories and this is a significant source of variability in the results of non-target screening exercises. The same sample can be shipped to multiple labs and each will return vastly different results. This is apparent in the results of numerous non-target trials to date.

NORMAN members have participated in several “non-target” trials, but the impact of deconvolution and library search algorithms have not yet been evaluated independently. We therefore propose this small project to make this evaluation. This project will increase our understanding of the different data processing tools used today and provide a platform to evaluate what can go wrong and why.

Description of the proposed activity and expected outcomes for 2018/2019:

All participants will be sent the following: a well-characterized sample-extract, guidelines on the required instrumental acquisition parameters, a target-list of features (i.e. retention time and m/z value pairs). Participants will be requested to run the samples in data independent mode and perform identification via their regular data processing tools. Final reports and the raw data will be submitted to the project coordinators.

This exercise will provide the opportunity to compare the performance of different deconvolution and library search algorithms. The results will be used to prepare a best-practice guideline for the NORMAN network, and a scientific paper for wider distribution.

Deadline for registration:

If you are interested in participating in the trial, please contact Saer Samanipour [saer.samanipour@niva.no] **before 1st of November 2018.**

Expert Meeting:

The expert meeting for this project will be combined with the meeting of the passive sampling working group on **November 28th in Thessaloniki, in conjunction with the Norman GA.** Details regarding the exact time and location of the meeting will be provided closer to the meeting.