

## Proposals for NORMAN Joint Programme of Activities 2022

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| <b>Title</b>                                       | <b>Data management of interlaboratory comparison on (semi-)quantitative non-targeted analysis with LC/ESI/HRMS</b>   |
| <b>Type of activity</b>                            | Data processing, database and dashboard building   |
| <b>Leader</b>                                      | Anneli Krueve (Stockholm University) and Nikolaos S. Thomaidis (University of Athens)  |
| <b>Topic / activities</b>                          | <p><b>Background / Justification for the proposed activity:</b></p> <p>This proposal is a continuation of the NORMAN JPA2020 activity "Collaborative trial on (semi-) quantitative non-targeted analysis with LC/ESI/HRMS". In October 2021, nine water samples were sent to 46 laboratories around the world for the above-mentioned interlaboratory comparison. The interlaboratory comparison tests 5 semi-quantification approaches and collects data on three levels: (1) semi-quantification results; (2) integration data; and (3) raw data. The data will be received from the laboratories in winter 2022. The data, however, does not speak for itself and needs to be managed to enable findability, accessibility, interoperability, and reusability (FAIR). In the continuation we will analyze the results from the collaborative trial and organize the data in a FAIR way. The data processing will be transparent and reproducible and is expected not only to find the most precise methods but will be used as a source for benchmarking future semi-quantification approaches. The best method will be integrated to the NORMAN Digital Sample Freezing Platform (DSFP) to improve suspect screening results and all related NORMAN activities (e.g. Prioritization of contaminants in context of WG1).</p> <p><b>Description of the proposed activities:</b></p> <p><b>Task 1:</b> Data curation, unification of the data processing between data from different labs, reintegrating the data if needed.</p> <p><b>Task 2:</b> Data analysis: comparison of the semi-quantification accuracy across methods, chemicals, instrument types, and analysis methods.</p> <p><b>Task 3:</b> Visualization of the result and creating an interactive dashboard for easy access to the results.</p> <p><b>Task 4:</b> Writing the publication, coordinating input from participating labs.</p> <p><b>Task 5:</b> Uploading and organizing the data, making data publicly available through NORMAN Digital Sample Freezing Platform.</p> <p><b>Task 6:</b> Integration of the most precise approaches to DSFP and NORMAN Database System.</p> <p><b>Added value / Link with other NORMAN activities and / or other projects</b></p> <p>It is a continuation of the JPA 2020 activity "Collaborative trial on (semi-) quantitative non-targeted analysis with LC/ESI/HRMS". The data will be curated, analysed, and made available and linked with NORMAN DSFP. Also, it will enable validation and possibly improvement of the ionization efficiency (log/E) values in the NORMAN SusDat and therefore aid exposure-based prioritization (WP1) of the compounds detected with NTS.</p> |
| <b>Participants</b>                                | Any interested parties   |
| <b>Proposed in-kind contribution</b>               | Tasks 2, 4, 5 and 6 (corresponds to 6-person month)  |
| <b>Contribution needed from NORMAN Association</b> | <p>Contribution with the data form the interlaboratory comparison.</p> <p>8,000 EUR for a student working on the tasks 1 and 3 (Louise Malm).</p>  |