

# Analysis of Hanöbukten Sediment and Cod using a Non-target Approach

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## Credits

30-45

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## Background

Observations of declining environmental conditions in Hanöbukten, Sweden, were first observed in 2010 by local fisherman, who reported reduced fish populations, fish wounds, and discolored, foaming or odorous water in this area. Subsequent investigations identified surface runoff, landfills, agriculture and forestry, and municipal wastewater treatment plants as potential sources of environmental contamination [1]. While monitoring campaigns have detected a suite of chemical contaminants in this area, no one substance has been identified as the major contributor to the observed deterioration in regional environmental quality.

In early 2017, ACES applied a non-target screening approach to Hanöbukten cod and sediments in an effort to elucidate potential chemical contaminants which would normally be missed by targeted analytical approaches. The approach involved a broad extraction procedure followed by analysis by high resolution (Orbitrap) mass spectrometry, which generates several thousand unique chromatographic features. The resulting dataset is a list of exact masses and relative intensities present in the Hanöbukten samples.

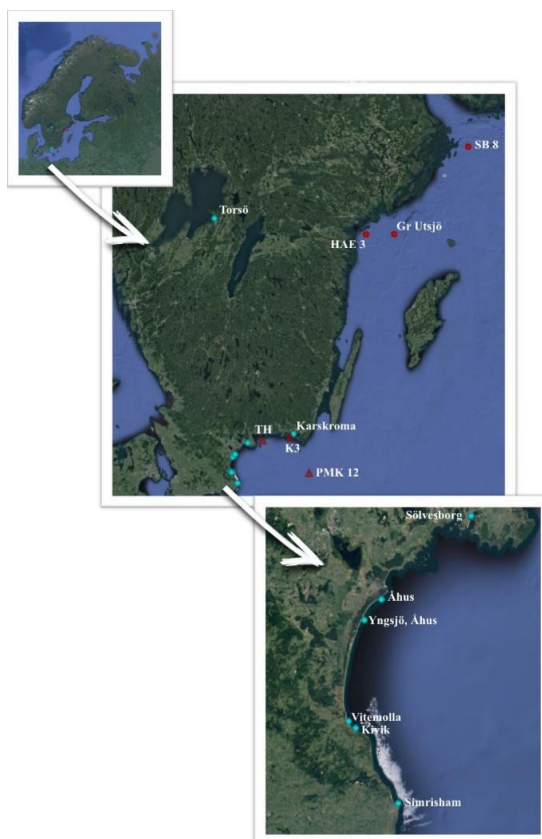
## Research Objectives

The current project is envisaged as a 30-45 credit Master's thesis, aimed at extracting further information from the Hanöbukten dataset. The overall objective is to unequivocally identify substances which are present in Hanöbukten sediments and cod but that are not observed in control sites. The project is divided into the following 3 parts:

- 1) Sequence correction of the Hanöbukten dataset using the R package 'batchCorr' [2].

2) Multivariate statistical analysis and database mining to identify features of interest in both sediment and cod.

3) Verification of tentative IDs via analysis of standards by UHPLC-Orbitrap-MS.



**Figure 1.** Sediment sampling locations are denoted by red markers (circles refer to reference samples and triangles to the study site) while fish sampling sites are denoted by blue markers.

### Training Objectives

- Gain hands-on experience in ultra-high performance liquid chromatography-high resolution (Orbitrap) mass spectrometry.
- Gain experience applying R-scripts for sequence correction of non-target data.
- Gain experience in the lab preparing samples and processing data.

### Methods

The R package ‘batchCorr’ will be used for sequence correction, after which missing value imputation, data normalization, and multivariate statistics will be carried out using MetaboAnalyst. Database mining will involve a combination of the Fisher database, MZCloud, ChemSpider, and others. Follow up confirmation of tentative structures will be carried out by analysing standards and sample extracts by UHPLC-Orbitrap-MS.

### References

[1] Hanöbukten, Regeringsuppdrag, Havs- och vattenmyndighetens rapport 2013-10-31(<https://www.havochvatten.se/download/18.5f66a4e81416b5e51f72d09/1383213915017/hanobuksutredningen-rapport.pdf>, last visited April 2017).

[2] Brunius et al. 2016 Large-scale untargeted LC-MS metabolomics data correction using between-batch feature alignment and cluster-based within-batch signal intensity drift correction. *Metabolomics*, 12, 173.