National Doctoral Program in Informational and Structural Biology

ISB Website, Abstract Submission

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Note that the abstract will be placed on the ISB website and will thus be public information. Students: please check with your supervisor before submitting.

B. Project title

Chemometric and metabolomics course Kuopio 30/08-3/09 2010

C. Abstract

The course was organized in the University of Eastern Finland more exactly in Kuopio from the 30th of August to the 3rd of September by Professor Seppo Auriola.

The course from my point of view was very interesting and complete. I would warmly suggest it to other PhD students that have to work with chemometrics and/or metabolomics.

It was a quite international course we had two international speakers, two speakers from finnish companies and a post doc from University of Kuopio.

The first two days we had a presentation on PCA and PLC from an assistant professor: Thomas Skov from the Spectroscopy and Chemometrics Group, University of Copenhagen. Both of the afternoons we had tutorial using the program LatentiX. For these two days we had plenty of material and course was very clear, going through the basics of PCA and PLC, how to notice

outliers and how to validate a PLC model. Wednesday Kati Hanhineva from University of Estern Finland, Kuopio started to define metabolomics, what it is and how to deal with the enormous quantity of data. In the afternoon we had some more tutorials and hand on exercises with Sanni Matero (post doc with experience in chemometrics). On Thursday we had a speaker from FIMM Dr Velagapudi that was presenting her work: how to use metabolomics data and how to understand it. In the afternoon two scientists from Agilent Technologies presented there software for dealing with metabolomics data, then we used the program. Finally Friday Matej Oresic from VTT, Espoo give us some good examples of how to use metabolomics in medicine and how he used it in his research.

We had to write a short assay on a project that we had carried on during the course. They give us spectroscopy data of wine and the relative concentration in ethanol. We had then to predict the concentration of ethanol of another set of data where this concentration was not determinate. For this we had to build a PLC model commenting all the steps, defining the outliers and the cross validation used. Our assays were then commented by Thomas Skov and Sanni Matero.

D. Date

24 September,2010

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