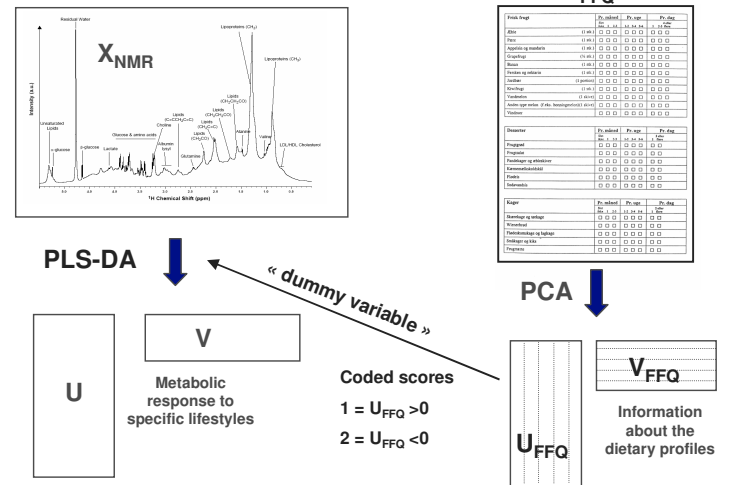


Introduction

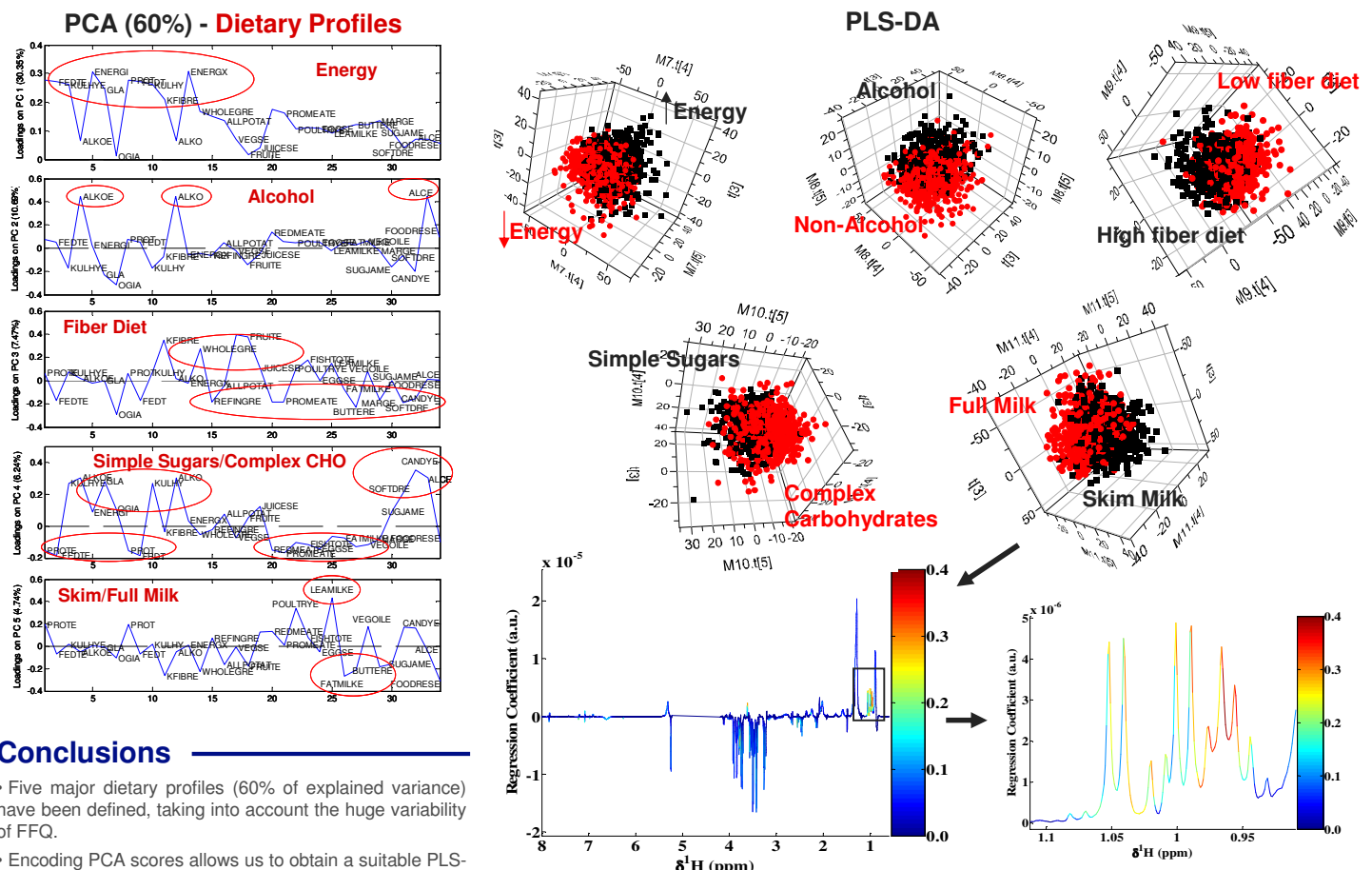
Application of metabolomics to nutritional sciences, also termed as nutrimetabolomics¹, offers a unique opportunity to measure metabolic responses associated with the consumption of specific nutrients and foods. Although metabolomics proved successful in toxicity screening¹, its application to nutrition sciences has been slow due to the fact that food generates subtle metabolic changes. This is an opportunity for developing an appropriate chemometric^{2,3} strategy to improve recovery of biological information in relation to different dietary habits. Data fusion, defined as “combination of information from different sources to produce a single model or decision”⁴, have been already applied to find biomarkers related to age, gender, BMI or different lifestyles⁵.

In this work we explore different approaches to combine the information from ¹H NMR data of plasma (CMPG spectra) and FFQ (Food Frequency Questionnaires).

Chemometrics



Results



Conclusions

- Five major dietary profiles (60% of explained variance) have been defined, taking into account the huge variability of FFQ.
- Encoding PCA scores allows us to obtain a suitable PLS-DA model according with the information present in FFQ.
- Samples are ordered in the space showing some non-random tendencies. As expected, there is an overlapping region between the two classes.
- Key biomarkers of energy metabolism were associated with specific dietary habits. Further work is required to better understand the metabolite correlations/interactions and to improve interpretation.

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Further Work

- Biomarker identification and nutrimetabolomics interpretation.
- Application of MCR-ALS with constraints to FFQ-data will be also performed to better define the dietary profiles.
- “Extreme samples” will be studied to facilitate data interpretation.

Acknowledgements

- NMR team
- Metabolomics and Biomarkers group
- Institute of Preventive Medicine, Denmark
- University of Southern Denmark