FWF Der Wissenschaftsfonds.

# Doctoral College
# Metabolic & Cardiovascular Disease

Medical University of Graz

UNI GRAZ TU Graz Graz University of Technology

# PRESENT AND FUTUR OF METABOLOMICS BY NMR

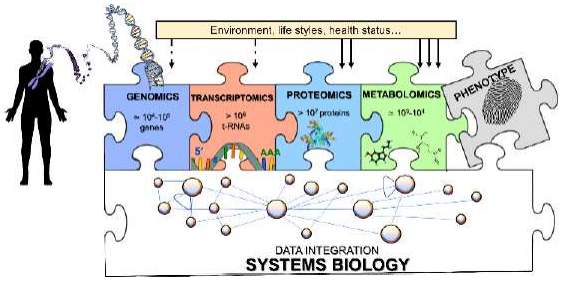
**GUEST LECTURE by**

## Prof. Dr. Claudio Luchinat

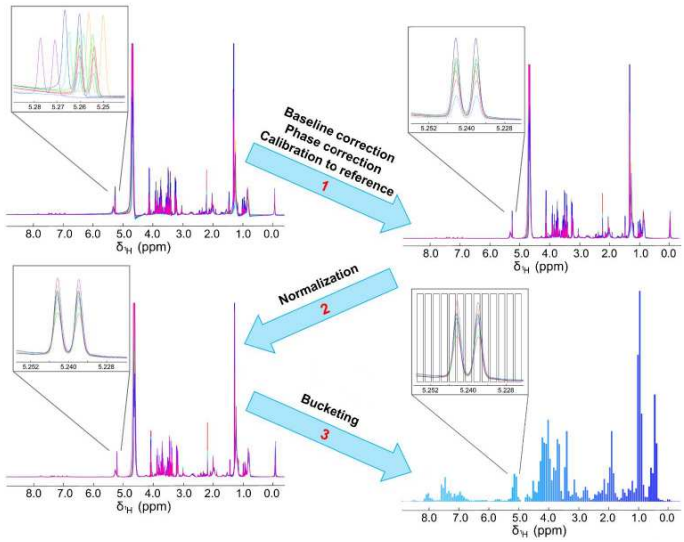
**Center of Magnetic Resonance (CERM)**
**and Department of Chemistry,**
**University of Florence, Italy**

## Friday, 05.10.2018
## 10:00

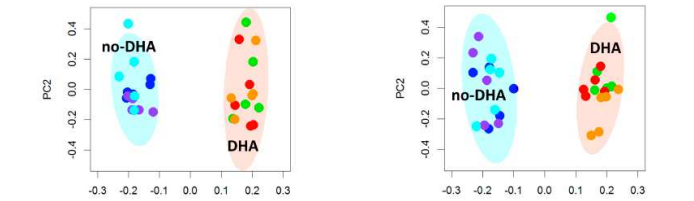
**Lecture Hall MC.05, MED Campus**
**(Neue Stiftingtalstrasse 6, ground floor), MUG**




The flow of information in systems biology
from „High-throughput metabolomics by 1D NMR."
Vignoli et al. (2018) Angew Chem Int Ed Engl. in press




Key stages of NMR spectral processing.
from „High-throughput metabolomics by 1D NMR."
Vignoli et al. (2018) Angew Chem Int Ed Engl. in press




| Confusion Matrix | | |
|---|---|---|
| P / A | DHA | No-DHA |
| DHA | 93.3 | 6.7 |
| No-DHA | 13.3 | 86.7 |

Discrimination accuracy = 90%

(a)

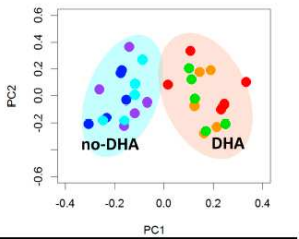



| Confusion Matrix | | |
|---|---|---|
| P / A | DHA | No-DHA |
| DHA | 100 | 0 |
| No-DHA | 0 | 100 |

Discrimination accuracy = 100%

(b)

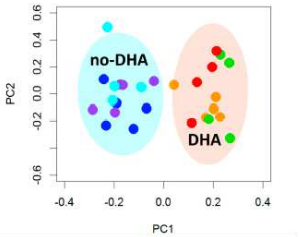
Lipidomic phenotyping by NMR analysis.
from „Evidence of a DHA Signature in the Lipidome and Metabolome of Human Hepatocytes."
Ghini et al. (2017) Int J Mol Sci. 18(2). pii: E359




| Confusion Matrix | | |
|---|---|---|
| A / P | DHA | no-DHA |
| DHA | 86.7 | 13.3 |
| no-DHA | 6.7 | 93.3 |

Discrimination accuracy = 90%

(a)




| Confusion Matrix | | |
|---|---|---|
| A / P | DHA | no-DHA |
| DHA | 92.9 | 7.1 |
| no-DHA | 7.7 | 92.3 |

Discrimination accuracy = 92.6%

(b)

Cytoplasmic metabolomic phenotyping by NMR analysis.
from „Evidence of a DHA Signature in the Lipidome and Metabolome of Human Hepatocytes."
Ghini et al. (2017) Int J Mol Sci. 18(2). pii: E359