

# Metabolomics

Objective: To give a presentation of about 60 minutes at the end of the week covering the key aspects of integrative genomics, which is the combined analysis of data from multiple sources/levels.

The questions and contents below are meant as motivators and need not be followed. Since we give several lectures on IG, you should probably try to give a new angle in the presentation or focus on a few new and exciting publications.

## The Big Questions Are:

- What are the key classes of data (OMICS)?
- What is the inherent variation in metabolomics?
- What was the first metabolomics investigation?
- Which omics classes are often combined in analysis?
- What is the largest metabolomics studies to data?
- Which models are used to analyze data?
- What is the dimensions of data?
- What is the methodological differences between metabolomics and proteomics?

***Recommended literature is only meant to get you started. You might very well be able to find papers more suited for your purpose.***

Davies, Rafnar, Hellenthal and Hein (2009) "Integrative Genomics and Functional Explanation" downloadable from <http://www.stats.ox.ac.uk/research/genome/publications>

Sreekumar et al. (2009) "Metabolomic profiles delineate potential role for sarcosine in prostate cancer progression" Nature 457. 910-15

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Lindon et al. (2005) Metabolomics in pharmaceutical R&D. Thermo Scientific, What is Metabolomics?.

Brown et al. (2004) A metabolome pipeline : from concept to data to knowledge

Trygg et al. (2006) Chemometrics in Metabolomics.

Lindon JC, Nicholson JK, 2008 Spectroscopic and Statistical Techniques for Information Recovery in Metabolomics and Metabolomics.

Scholz M, Fiehn O, 2007, SetupX: A public study design database for metabolomic projects.

Markley et al. (2002) New bioinformatics resources for metabolomics.

Holmes E, Antti H, (2002) Chemometric contributions to the evolution of metabolomics:

mathematical solutions to characterising and interpreting complex biological NMR spectras.

Scott R, et al. (2008) Noninvasive metabolomic profiling of human embryo culture media using Raman spectroscopy predicts embryonic reproductive potential: a prospective blinded pilot study. Fertility and Sterility, 2008. Fertil Steril. 2008 Jul;90(1):77-83.

Botros et al. 2008) Metabolomics and its application for non-invasive embryo assessment in IVF, Molecular Human Reproduction 2008 14(12):679-690

Seli et al. Noninvasive metabolomic profiling of human embryo culture media using proton nuclear magnetic resonance correlates with the reproductive potential of embryos of women undergoing in vitro fertilization. Fertility and Sterility, Volume 90, Issue 6, Pages 2183-2189

Vergouw et al. (2008) Metabolomic profiling by near-infrared spectroscopy as a tool to assess embryo viability: a novel, non-invasive method for embryo selection, Human Reproduction 2008 23(7):1499-1504

Seli, MD, A New Method for Embryo Selection: Metabolomics

Sreekumar et al. (2009) Metabolomic profiles delineate potential role for sarcosine in prostate cancer progression; Nature 457, 910-914

David S. Wishart, 2007, Current Progress in computational metabolomics

Rennie et al. The Metabolic Effect on Strenuous Exercise: A Comparison between Untrained Subjects and

Racing Cyclists Medical Sciences 59.3 pp 201-212

Seli et al. Noninvasive metabolomic profiling of embryo culture media using Raman and near-infrared spectroscopy correlates with reproductive potential of embryos in women undergoing in vitro fertilization; Fertility and Sterility, Volume 88, Issue 5, Pages 1350-1357

Spectroscopic and Statistical Techniques for Information Recovery in Metabolomics and Metabolomics John C. Lindon and Jeremy K. Nicholson

Nicholson JK, Wilson ID. 1989. High-resolution proton magnetic resonance spectroscopy of biological fluids. Prog. NMR Spectrosc. 21:449-501

van der Greef et al. (1983) Evaluation of elution-desorption and fast atom bombardment mass spectrometric profiles by pattern-recognition techniques. Anal. Chim. Acta 150:455