

Workshop on Metabolomics and Chemometrics

16th of November 2015, Ein Gedi, Israel (8:30am – 5:30 pm)



1. Metabolomics

1.1 Introduction to Metabolomics (8:30 – 9:00)

1.2 Metabolomics study design (9:05 – 9:50) (10 min break)

1.3 Standard Operating Procedures for Metabolomics (10:00 – 10:30)

1.4 Choice of Analytical Platform (GC-MS, NMR, LC-, CE- , SFC-MS, LC-MS-SPE-NMR) (10:35 – 11:30)

1.5 Metabolite Identification (level 1, 2, 3) (11:30 – 12:00)

Lunch (12:00 – 13:00)

1.6 Team Work (questioner, DoE task (13:00 – 13:25)

1.7 Metabolomics Data Handling (13:30 – 13:55)

1.8 Introduction to PARAFAC2 and hands on PARAllel FACtor Analysis2 based Deconvolution and Identification System (PARADISE) (14:00 – 14:50) (10 min break)

2. Chemometrics

2.1 Introduction to Multivariate Data Analysis (15:00 – 15:20)

2.2 Data pre-processing (15:25 – 15:45)

2.3 Unsupervised Methods, Principal Component Analysis (PCA) (15:50 – 16:05)

2.4 Supervised Methods, Partial Least Squares (PLS) Regression Analysis and PLS- Discriminant Analysis (PLS-DA) (16:10 – 16:30)

2.5 Introduction to LatentiX and hands on PCA and PLS using LatentiX (16:45 – 17:30)

Note: Lecture times may slightly change